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Michael E. DUNN[1,*] and Luiz C. LEAL[1]

[1]*Computational Physics and Engineering Division, Oak Ridge National Laboratory,*[**]
P. O. Box 2008, Oak Ridge, TN 37831-6370, USA

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*Corresponding author, Tel. (865) 574-5260, Fax. (865) 576-3513
E-mail: dunnme@ornl.gov and leallc@ornl.gov

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A Monte Carlo Approach to Calculate Probability Tables for the Unresolved-Resonance Region Using the AMPX Cross-Section Processing System

Michael E. DUNN[1,*] and Luiz C. LEAL[1]

[1]*Computational Physics and Engineering Division, Oak Ridge National Laboratory, P. O. Box 2008 Oak Ridge, TN 37831-6370, USA*

A new module, PURM (**P**robability tables for the **U**nresolved **R**egion using **M**onte Carlo), has been developed for the AMPX-2000 cross-section processing system. PURM uses a Monte Carlo approach to calculate probability tables on an evaluator-defined energy grid in the unresolved-resonance region. For each probability table, PURM samples a Wigner spacing distribution for pairs of resonances surrounding the reference energy. The resonance distribution is sampled for each spin sequence (i.e., ℓ-J pair), and PURM uses the Δ_3-statistics test to determine the number of resonances to sample for each spin sequence. For each resonance, PURM samples the resonance widths from a Chi-square distribution for a specified number of degrees of freedom. Once the resonance parameters are sampled, PURM calculates the total, capture, fission and scatter cross sections at the reference energy using the single-level Breit-Wigner formalism with appropriate treatment for temperature effects. Probability tables have been calculated and compared with NJOY. The probability tables and cross-section values that are calculated by PURM and NJOY are in agreement, and the verification studies with NJOY establish the computational capability for generating probability tables using the new AMPX module PURM.

KEYWORDS: probability tables, unresolved-resonance region, Monte Carlo, cross section, AMPX

I. Introduction

In the United States, the Evaluated Nuclear Data File (ENDF) system [1)] is the repository for evaluated cross-section data. The AMPX-2000 code system, which is maintained at the Oak Ridge National Laboratory (ORNL), is used to process ENDF evaluations and generate continuous-energy and multigroup cross-section libraries. 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; however, the values of the parameters vary as a function of the different energy intervals. Because of 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 have been used to generate probability tables for an isotope of interest. The conventional or 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. This process is then repeated over additional ladders of resonances until the desired number of ladders is processed. The ladder approach, which is described by Levitt,[2)] is the basis for the probability-table method in NJOY.[3)]

A new and different procedure relative to the "ladder" approach is used in the AMPX cross-section processing system that has been developed at ORNL. A new AMPX module, PURM has been developed to calculate probability tables in the URR using Monte Carlo (MC) procedures. The objective of this work is to demonstrate the capability for calculating probability tables using PURM.

II. Methodology

The objective of the probability-table method is to calculate a distribution function for the cross-section values in a specific energy range within the URR. The approach is in direct contrast with the procedures of the resolved-resonance region (RRR) in which the neutron cross section is obtained at a specific energy using the appropriate resonance formula. The cross-section distribution function is characterized by having a mean value that is equivalent to the infinite-dilution cross-section value for the energy range of interest.

1. Resonance-parameter Sampling

PURM uses a MC procedure to calculate probability tables on the evaluator-defined energy grid in the unresolved region. The MC procedure used in PURM is based on the methodology of the code URR[4)] that was developed at ORNL in the late 1980s. As opposed to generating a ladder of resonances, PURM determines pairs of resonances or levels

*Corresponding author, Tel. (865) 574-5260, Fax. (865) 576-3513
E-mail: dunnme@ornl.gov and leallc@ornl.gov

surrounding the reference energy or energies for each table. As in the ladder approach, the level spacings are sampled from a Wigner distribution:

$$f(x) = W(x) = \frac{\pi}{2} x\, e^{-\frac{\pi}{4}x^2}, \qquad (1)$$

where x is the ratio of the level spacing to the mean level spacing provided in the ENDF data. The resonance and mean level spacing are denoted as $D_{\ell,J}$ and $< D_{\ell,J} >$, respectively, for relative neutron-nucleus angular momentum, ℓ, and resonance spin, J. The spacing distribution in Eq. (1) is a probability density function (PDF) that is normalized to 1. In order to sample the level spacing for a specific ℓ-J series of resonances (i.e., $D_{\ell,J}$), the PDF is converted to a cumulative distribution function (CDF) by integrating Equation (1) from 0 to x. The value of x is obtained by setting the CDF equal to a random number, R, between 0 and 1. After solving for x, the resonance spacing is calculated as the product of x and $< D_{\ell,J} >$.

Once the spacing is sampled from the Wigner distribution, the position, x', of the reference energy in the spacing is selected from a uniform distribution (i.e., $x' = R\, D_{\ell,J}$). The positions of the first and second resonances relative to the reference energy, E_0, are obtained by the following expressions:

$$E_{\lambda=1} = E_0 + x', \qquad (2)$$

and

$$E_{\lambda=2} = E_0 + x' - D_{\ell,J}. \qquad (3)$$

The first pair of resonances that are located above and below the reference energy is determined by Eqs. (2) and (3), respectively. For the remaining pairs of resonances to be processed, the resonance spacings are sampled from the Wigner distribution, and the location of the resonances are determined using a procedure that is analogous to the steps for the first pair of resonances. Although the procedure for sampling the resonance spacing is straightforward, the code must determine the appropriate number of pairs of resonances to sample. To estimate the number of resonances to sample, PURM uses the Δ_3-statistics test which is described in Section II.2.

Once the distribution of energy levels is sampled, the resonance widths must be sampled for each resonance. In the unresolved region, the ENDF data provide average widths for reference energies in the URR. The distribution function for the resonance widths follows a Chi-square distribution with a designated number of degrees of freedom, ν:

$$P_\nu(y) = \frac{\nu}{2G(\nu/2)} (\nu y/2)^{\frac{\nu}{2}-1} e^{-\nu y/2}, \qquad (4)$$

where y is the ratio of the resonance width for a particular channel (i.e., $\Gamma_{\lambda c}$) to the mean channel width for a given energy range (i.e., $<\Gamma_{\lambda c}>$). The different channels, c, that are considered are fission, capture and scattering. In Eq. (4), the quantity $G(\nu/2)$ is the mathematical gamma function. For the neutron width, ν is typically equal to 1, and Equation (4) has the form of the Porter-Thomas distribution law of the neutron width.[5, 6] Fission is regarded as a few-channel process, and two or three degrees of freedom (ν = 2 or 3) are typically assumed for the fission width distribution. Regarding neutron capture, there are a large number of capture channels that are available, and the number of degrees of freedom is assumed to approach infinity ($\nu \to \infty$), and the Chi-square distribution becomes a Dirac-delta function centered at $\Gamma_{\lambda\gamma} = < \Gamma >$. As noted previously, the ENDF data provide the average resonance widths along with the number of degrees of freedom for the corresponding Chi-square distribution. During the MC simulation, PURM obtains the widths for each resonance by sampling the Chi-square distribution with the corresponding number of degrees of freedom.

The sampled widths and spacings are used to calculate cross sections in the URR using the single-level Breit-Wigner (SLBW) formulae. PURM has the capability to calculate temperature-dependent cross sections in the unresolved region. The sampled resonance parameters are used in conjunction with the SLBW formulae to calculate temperature-dependent cross sections for scattering, capture, fission and total. The SLBW formulae[4] are well documented and not presented in this paper. Note that the temperature dependence of the cross sections are obtained using the symmetric and antisymmetric-line-shape functions (i.e., ψ and χ, respectively) that are documented in most reactor theory textbooks.

2. Dyson and Mehta Δ_3-Statistics Test

One of the essential tasks for constructing the resonance distribution for a given spin sequence (i.e., ℓ-J pair) is the determination of the appropriate number of pairs of resonances to process. A useful tool for evaluating the distribution of resonances is the Δ_3-statistics test that was developed by Dyson and Mehta.[5, 7] PURM uses the Δ_3-test to determine the appropriate number of pairs of resonances to process for each spin sequence.

The Δ_3-test provides a measure of the mean-square deviation between the number of observed energy levels within an energy interval from E_i to E_f:[7]

$$\Delta_3 = Min(a,b)\left[\frac{1}{2L}\int_{E_i}^{E_f} (N(E) - aE - b)^2 dE\right], \qquad (5)$$

where $2L$ is the total number of resonances and $N(E)$ is the

observed cumulative number of resonances as a function of energy. In Eq. (5), *a* and *b* are the slope and constant, respectively, for a linear fit to the observed cumulative number of resonances as a function of energy.

The numerical procedures that are provided in Ref. 5 for calculating Δ_3 for a spin sequence are used in PURM to evaluate the expression in Eq. (5). For the sampled distribution of resonances for each spin sequence, PURM calculates a Δ_3 value and the linear fit for the cumulative number of levels (i.e., $N(E) = aE + b$). The Dyson and Mehta Δ_3-test also predicts that the theoretical average value for Δ_3 is given by the following expression:

$$<\Delta_3> = \frac{1}{\pi^2}[\ln(n) - 0.0687] , \qquad (6)$$

where *n* is the number of energy levels observed in the interval from E_i to E_f. The variance of $<\Delta_3>$ is $1.169/\pi^4$.

The objective of the Δ_3-test is to determine a resonance spacing distribution that provides a Δ_3 value that is in agreement with $<\Delta_3>$. In addition to the comparison between the calculated and theoretical values for Δ_3, the linear fit for the cumulative number of levels should agree with the observed number of levels in the sampled distribution.

There is a two-part convergence problem for the implementation of the Δ_3-statistics test. One part involves the linear fit for $N(E)$ as a function of energy, and the second part involves the convergence of the Δ_3 values. In other words, reasonable Δ_3 values (i.e., within 2 standard deviations of theoretical value) may be obtained for a sampled distribution; however, the cumulative number of resonances that is predicted by the linear fit may not correspond to the observed number of resonances for the distribution. In contrast, an acceptable linear fit for the cumulative number of resonances may be obtained for a sampled distribution, but the Δ_3 value for the sampled distribution may disagree with the theoretical value by more than two standard deviations. The Δ_3 test is extremely sensitive to the location of each level in the distribution.

Regarding implementation of the Δ_3 test, PURM determines the number of levels to sample for each spin state based on a linear fit for the cumulative number of observed levels. In other words, PURM samples a Wigner distribution to obtain a distribution of resonances using some initial value for the pairs of resonances to sample about the reference energy. The linear fit for the cumulative number of levels is compared with the observed number of levels in the sampled distribution. The number of pairs of resonances to sample is incremented until the observed number of levels in the sampled distribution is predicted to within 0.1% by the linear fit for $N(E)$. The Δ_3 value is also calculated for the sampled distribution; however, PURM currently does not attempt to find a resonance distribution that has a Δ_3 value within two standard deviations of the theoretical value as well as an acceptable linear fit for the cumulative number of levels. Extensive CPU times would be required to seek convergence for both the Δ_3 value and an acceptable fit for the cumulative number of levels. PURM searches for the distribution that provides an acceptable linear fit for the cumulative number of levels. Based on calculational experience, accurate cross-section values can be obtained by seeking convergence for the cumulative number of levels.

3. Monte Carlo Simulation

Because the URR is an energy region where the parameters are averages of resolved-resonance parameters over an evaluator-defined energy region within the URR, MC procedures can be used to calculate the average cross sections within the URR. Since random variables are used in the sampling procedures for the resonance parameters, different resonance parameters and cross sections can be obtained from different random number sequences. However, the MC simulation of the problem can estimate the desired cross-section quantity by observing the behavior of a large number of individual histories.* The exact solution can be approximated if a sufficiently large number of histories are processed. This concept is often referred to as The Law of Large Numbers.

For the purposes of discussion, a single history or i^{th} estimate of a cross-section quantity is denoted as $\sigma_{c\,i}$, where *c* denotes either total, capture fission or scatter. For each history, pairs of resonances are randomly sampled for each ℓ-*J* spin sequence, and the number of resonances is determined using the Δ_3-statistics test. For each resonance, the partial widths are sampled from a Chi-square distribution as defined by Eq. (4). The resonances and corresponding widths are sampled for each ℓ-*J* spin sequence. The i^{th} estimates for the capture, fission and scatter cross sections are obtained using the SLBW formulae and summing the contribution from all ℓ and *J* states. The i^{th} estimate for the total is obtained by summing the capture, fission and scatter cross section. The process is repeated for each history until *n* histories have been processed. The MC estimate of the mean cross-section value is given by the following expression with the reaction identifier, *c*, implied in the expression:

$$\bar{\sigma}_j = \frac{1}{n}\sum_{i=1}^{n} \sigma_i . \qquad (7)$$

Note that the definition of *j* will be provided shortly. The value of $\bar{\sigma}_j$ will approach the true mean as *n* approaches ∞. The variance of $\bar{\sigma}_j$ is estimated with the following expression:

$$V^2_{\bar{\sigma}_j} = \frac{1}{n(n-1)}\sum_{i=1}^{n} (\sigma_i - \bar{\sigma}_j)^2 . \qquad (8)$$

In Eq. (7), the value of $\bar{\sigma}_j$ is obtained from *n* estimates of

*A history denotes a single calculation or estimate of the total cross-section at an energy *E* from the sampled resonances and corresponding widths. Note that the capture, fission and scatter cross sections are also calculated as part of a single history.

the mean value. Let the quantity defined by Eq. (7) constitute a "batch" estimate of the mean value. Using the batch terminology, the j^{th}-batch estimate for the mean value is denoted with the subscript j in Eq. (7). If a different set or batch of n random samples is taken, a different mean cross-section value would be calculated. Based on the Central Limit Theorem,[8] if N batch estimates for $\bar{\sigma}_j$ are obtained, the distribution of $\bar{\sigma}_j$ will approach a normal distribution as N increases. The Central Limit Theorem implies that the statistical nature of the distribution of $\bar{\sigma}_j$ is independent of the actual distribution of the individual samples (i.e., σ_i). If N batches are processed, the "grand mean" is calculated by averaging over all the batches:

$$\bar{\sigma} = \frac{1}{N} \sum_{j=1}^{N} \bar{\sigma}_j \ . \qquad (9)$$

The variance is calculated with the following expression:

$$V_{\bar{\sigma}}^2 = \frac{1}{N(N-1)} \sum_{j=1}^{N} (\bar{\sigma}_j - \bar{\sigma})^2 \ . \qquad (10)$$

In PURM, the mean value for the total, capture, fission and scatter cross sections is obtained using Eq. (9) based on N batch estimates of each reaction.

Each probability table is constructed using monotonically increasing band limits (i.e., $B_1 < B_2 < ... < B_k < ... < B_K < B_{K+1}$) that are based on the total cross section. If K cross-section bands are defined, K+1 band limits are required to define the table. The band limits increase in value with a corresponding increase in band number. As a result, the lower cross-section band value for the first band is the minimum band value for the table, and the upper cross-section band value for the last band is the maximum band value for the table. Because the table construction is based on the total cross section, the average total cross-section value in each band should also increase monotonically with increasing band number. Note that the band averages for the corresponding partial reaction cross sections are conditional averages that correspond to the average total cross section for the band. Consequently, the band-average cross-section values for capture, fission and scatter will not necessarily increase monotonically.

In PURM, there are three options to determine the band values for each table. For the first option, the user can specify the band values for each table, and for the remaining two options, PURM can construct each table with either equal- or nonequal-probable cross-section bands. If nonequal-probable cross-section bands are used, the total cross-section band values are calculated with the following expression:

$$B_k = B_{\min} \left(\frac{B_{\max}}{B_{\min}} \right)^{\frac{k-2}{K-2}} \ ; \ k = 2,3,.....,K \ , \qquad (11)$$

where B_{min} is the lower bound for the second band, and B_{max} is the lower bound for the last band (i.e., B_K). The values of B_{min} and B_{max} can be specified by the user or determined by the code. If the user does not specify the values of B_{min} and B_{max}, PURM estimates these values. Once the values of B_{min} and B_{max} are established, PURM uses Eq. (11) to construct the cross-section band limits for each probability table. Note that B_1 and B_{K+1} are not determined prior to the calculation of a probability table. The values of B_1 and B_{K+1} represent the absolute minimum and maximum cross-section values of the MC simulation. As a result, the absolute minimum and maximum cross-section values are determined during the calculation of each probability table. The value of B_1 must be ≥ 0 and $< B_2$, and the value of B_{K+1} can be any value that is greater than B_K.

Once the cross-section band limits are established for a table, PURM performs a MC simulation for each table using a specified number of iterations or histories for a specified number of batches. For a single history in PURM, the procedures of Section II.1 and II.2 are used to sample the resonance parameters for the reference energy point in the URR. Subsequently, the SLBW formulae are used to calculate the scatter, capture, fission and total cross sections at the reference energy. As noted previously, the calculation of the total cross section and corresponding partial reactions at the reference energy constitute a single history.

For each history in a batch, the calculated total cross-section value is compared with the cross-section band limits for the table. The total cross-section is added to the appropriate cross-section band (i.e., k^{th} band) within the probability table. In addition, a counter assigned to the band is advanced by unity. The corresponding band values for the scatter, capture and fission cross sections are also added to the appropriate registers for the k^{th} band. Note that the band selection for the partial reactions is based on the value of the total cross section. At the completion of the number of histories for the batch, the average value for the total cross section for the k^{th} band (i.e., $\bar{\sigma}_{t,k}$) is calculated by dividing the cumulative sum for the band by the number of tallies within the band. The corresponding average band values for the scatter, capture and fission cross sections are calculated in a similar manner to the total cross section. The batch estimate for the probability for each band is obtained by dividing the number of tallies for the band by the number of histories in a batch. Once the initial batch is completed, the next batch is processed using the same procedure for each history in a batch. The calculation for a table is complete when all of the batches have been processed.

Due to the nature of the calculational procedures, PURM provides a mechanism for monitoring the convergence of the cross-section calculation. During the MC calculation for a table, PURM stores a "running" average (i.e., by batch processed) of the total, capture, fission and scatter cross section for the entire probability table. PURM has the capability to plot the cross-section calculation by batches run. Also, PURM provides histogram frequency plots for each calculation for a reaction and performs a test for normality for the MC calculation for each reaction.

III. Results

PURM has been used to calculate probability tables for ENDF/B-6 ^{235}U (MAT = 9228). Results are provided to demonstrate the capabilities of PURM. In addition, comparisons are made with the NJOY99.14 module PURR to verify the calculational results obtained with PURM.

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 total number of histories is relatively low compared with typical MC radiation transport calculations (e.g., deep-penetration shielding problems, eigenvalue calculations, etc.). Fortunately, probability-table calculations do not have the complexities that are associated with radiation transport problems (e.g., complex geometry, particle streaming, etc.). As a result, a probability table calculation is generally a well-behaved problem. Therefore, a relatively large number of histories is not required to obtain acceptable statistics in a probability-table calculation.

The PURM results for the probability table at 2.25 keV are presented in **Table 1**. For ^{235}U, the probability tables were calculated with 5 nonequal probable cross-section bands. The probability and standard deviation associated with each band are also provided in Table 1. Moreover, the average cross-section values and standard deviations for the total, capture, fission and scatter cross-sections are provided for each band within the probability table. PURM also provides the average cross-section values for each table, and the average values (in barns) for total, capture, fission and scatter are 19.68 ± 0.04, 2.04 ± 0.01, 5.70 ± 0.02 and 11.94 ± 0.01, respectively. Note that the average cross-section values for the table represent the infinite dilution values for ^{235}U at 2.25 keV and 300 K.

For each probability-table calculation, PURM provides the results of the Δ_3-statistics. The number of levels that is predicted from the Δ_3-statistics test are provided in **Table 2** for the ^{235}U calculation at 2.25 keV. In Table 2, the number of levels for the calculation is provided for each ℓ-J spin sequence. Note that the observed number of levels, which is obtained by iteration, are presented in Table 2. Based on the Δ_3-statistics test, the predicted number of levels, $N(E)$, is also provided for comparison. The value for $N(E)$ is obtained by performing the Δ_3-statistics analysis for the observed number of levels and corresponding spacing distribution. As shown in Table 2, the predicted values are within 0.01% of the observed number of levels in the MC calculation.

Table 2 Predicted Number of Levels from Δ_3-Statistics for ^{235}U at 2.25 keV

ℓ	J	Observed No. of Levels	$N(E)$	a	b
0	3.	727	727.01	1.02	-1.93×10^{3}
0	4.	895	895.05	1.28	-2.43×10^{3}
1	2.	538	537.94	0.76	-1.44×10^{3}
1	3.	717	717.03	1.02	-1.94×10^{3}
1	4.	889	889.03	1.26	-2.39×10^{3}
1	5.	997	997.0	1.41	-2.68×10^{3}

To help visualize the calculated results that are presented in Table 1, the probabilities as a function of the cross-section bands are plotted in **Fig. 1**. In addition, NJOY99.14 was used to calculate probability tables for ^{235}U at 300 K. The probabilities that are obtained with NJOY at 2.25 keV are also presented in Fig. 1. Based on the results in Fig. 1, the PURM-calculated probabilities agree with the NJOY values. Similar agreement is obtained for the NJOY and PURM average band values for the total, capture, fission and scatter cross sections. Note that similar results are also obtained for the remaining 13 probability-table calculations for ^{235}U. Based on the verification studies with NJOY, the probability tables as calculated by PURM are suitable for use in nuclear applications.

Table 1 Probability Table for ^{235}U at 2.25 keV and 300 K

Band	Limits[a]	Probability[b]	Total[a, b]	Capture[a, b]	Fission[a, b]	Scatter[a, b]
1	11.86	0.131 (0.003)	14.35 (0.02)	0.72 (0.01)	2.27 (0.02)	11.36 (0.02)
2	15.30	0.380 (0.005)	17.13 (0.02)	1.37 (0.01)	4.07 (0.02)	11.70 (0.01)
3	18.97	0.313 (0.005)	20.97 (0.03)	2.33 (0.02)	6.62 (0.02)	12.02 (0.01)
4	23.51	0.142 (0.003)	25.69 (0.04)	3.59 (0.05)	9.50 (0.06)	12.60 (0.03)
5	29.15	0.034 (0.002)	31.98 (0.16)	5.50 (0.13)	13.06 (0.20)	13.42 (0.09)
	56.28					

[a] Cross-section values are in barns

[b] Quantities in parentheses represent 1 standard deviation

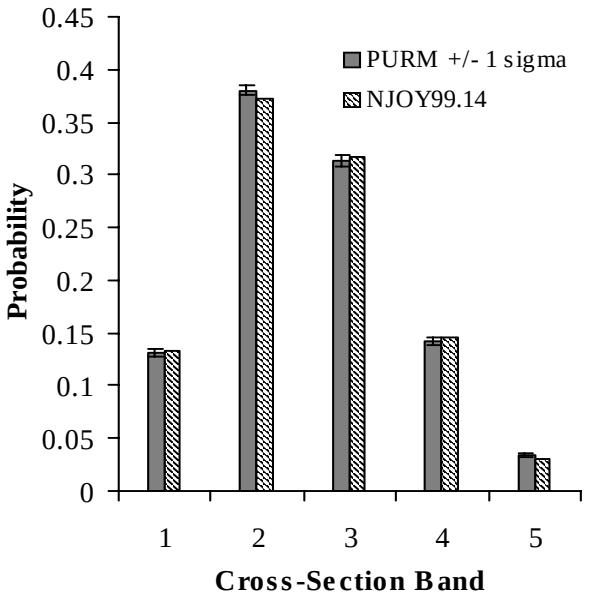

Fig. 1 Probability-table comparison between PURM and NJOY for ^{235}U at 2.25 keV and 300 K

IV. Summary

PURM is a Monte Carlo code that has been developed to calculate probability tables for the unresolved-resonance region. In an effort to establish the new procedures, probability tables have been calculated for ENDF/B-6 ^{235}U using PURM and NJOY. The probability tables and corresponding cross-section values obtained with both codes are in agreement. As a result, the verification studies establish the computational capability for generating probability tables using the new AMPX module PURM.

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