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Effect of Energy Self-Shielding Methods on ^{238}U for Criticality Safety Problems

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Multigroup cross sections are obtained by weighting point-wise nuclear data with a flux spectrum. For nuclides having a resonance structure, energy self-shielding calculations are performed to calculate a more detailed flux spectrum. Subsequently, self-shielded multigroup cross sections are generated. Different methods exist for energy self-shielding calculations. Among them are the Bondarenko method, NJOY flux calculator and the CENTRM method. The CENTRM method is a more advanced technique that utilizes both multigroup and point-wise cross sections in a one-dimensional transport calculation to solve for a point-wise flux distribution.

The method of energy self-shielding is one of the elements in a multigroup cross-section generation that may have a significant impact on the multiplication factor in criticality safety calculations. This paper compares the three aforementioned self-shielding methods applied to ^{238}U. A criticality problem having twenty-three cases is considered. This system includes water moderated, low enriched UO_2 fuel rods in square pitched array, with a thermal flux spectrum. Multiplication factors obtained from transport calculations that use multigroup and continuous energy data are compared. It is observed that multiplication factors calculated with multigroup data containing different self-shielding methods for ^{238}U have less than 500pcm difference with continuous energy results.

KEYWORDS: energy self-shielding, Bondarenko method, NJOY flux calculator, CENTRM, criticality safety benchmark, low-enriched Uranium fuel

1. Introduction

The NJOY code [1] is widely used for processing evaluated nuclear data to obtain point-wise or multigroup cross sections. Multigroup cross sections are generated by collapsing thousands of points processed from the evaluated data into energy groups that contain average cross-section values. Average cross sections are obtained by weighting points of data with a flux spectrum. The weighting flux may be chosen to be a smooth function of energy; e.g. a 1/E spectrum for the epithermal energy range. However, due to the cross-section behavior of some nuclides, using a smooth flux spectrum may not be a good choice. There are many isotopes having significant resonance structures in cross sections that need to be weighted with a detailed flux spectrum. The correction introduced in the flux spectrum to account for the resonance structure results in obtaining energy self-shielded cross sections.

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In this paper, three methods are utilized in NJOY for calculating the flux spectrum. These are: (i) the NJOY flux calculator [1], (ii) the Bondarenko method [1,2] and (iii) the CENTRM method [3,4]. In Section 2 these three methods are described. Section 3 compares the Bondarenko and flux calculator methods for ^{238}U considering self-shielding factors. In Section 4, different self-shielded multigroup ^{238}U cross sections are used in a criticality safety benchmark problem consisting of twenty-three cases. Multiplication factors are compared using multigroup and continuous energy data. Finally, Section 5 presents conclusions.

2. Methods Used in Self-Shielding Calculations

In this paper three self-shielding methods are analyzed. These methods are:

(i) The NJOY flux calculator
(ii) The Bondarenko method
(iii) The CENTRM method

2.1 The Flux Calculator

The infinite-medium neutron spectrum equation is expressed as:

$$\Sigma_t(E)\Phi(E) = \int_0^{\infty} dE' \Sigma_s(E' \rightarrow E)\Phi(E') + S(E) \tag{1}$$

where the term on the left hand side of the Equation (1) represents the collision, the integral on the right hand side is the scattering source, and S(E) is the external source.

Next, Equation (1) is written considering a homogeneous medium consisting of two materials: an absorber and a moderator, represented by *A* and *M*, respectively in Equation (2). Elastic scattering cross sections that are isotropic in the center of mass are used. Neutron slowing down in a single resonance of the absorber material is assumed.

$$\Sigma_t(E)\Phi(E) = \int_E^{E/\alpha_M} dE' \frac{\Sigma_s^M(E')}{(1-\alpha_M)E'}\Phi(E') + \int_E^{E/\alpha_A} dE' \frac{\Sigma_s^A(E')}{(1-\alpha_A)E'}\Phi(E') \tag{2}$$

where α_M and α_A are the moderator and absorber collision parameters, respectively, defined as:

$$\alpha = \left(\frac{A-1}{A+1}\right)^2 \tag{3}$$

A is the atomic mass in Equation (3)

The following approximations are introduced to Equation (2):

- The moderator scattering cross-section is assumed to be constant and equal to the potential scattering cross-section; i.e. $\Sigma_s^M(E') = \Sigma_p^M$

- The moderator absorption cross-section is assumed to be negligible; i.e. $\Sigma_t^M(E') = \Sigma_p^M$

- The narrow resonance approximation is used for the moderator. This states that the resonance width is very small compared to the energy loss from scattering with the moderator nucleus. Therefore, the flux distribution in the moderator integral is assumed to have an asymptotic form. In general, the moderator integral is assumed to be a smooth function of energy represented as C(E).

- The moderator is assumed to represent all nuclides other than the absorber. This enables the inclusion of the dilution microscopic cross-section of the absorber, σ_o, in Equation (2). The dilution (or background) cross-section of an isotope *i* is defined to be all cross sections representing isotopes other than the isotope *i*. The dilution cross-section is a measure of energy self-shielding. It determines the significance of a resonance compared to other cross

sections. If the dilution cross-section (σ_o) is small, it indicates that the resonance has a significant impact on the flux and a large self-shielding effect exists. If σ_o is very large (infinite dilution), the cross sections of the absorber do not effect the flux spectrum, and the flux may be represented as a smooth function of energy.

Including the above approximations, Equation (2) becomes:

$$\left[\sigma_o + \sigma_t^A(E)\right]\Phi(E) = C(E)\sigma_o + \int_E^{E/\alpha_A} dE' \frac{\sigma_s^A(E')}{(1-\alpha_A)E'}\Phi(E') \tag{4}$$

The dilution cross-section for an isotope *i* is given as:

$$\sigma_o = \frac{1}{\rho_i}\sum_{j\neq i}\rho_j\sigma_t^j \tag{5}$$

where *i* and *j* represent isotope indexes and ρ is atomic density.

Equation (4) is the simplest form used in NJOY for computing the flux with the flux calculator option. In NJOY, several dilution cross sections are provided as input. Depending on a system of interest, the cross sections corresponding to the appropriate dilution cross-section are used.

2.2 The Bondarenko Method

The Bondarenko method is obtained by using the narrow resonance approximation in the absorber integral of Equation (4). The practical width of a resonance of the absorber is considered to be much smaller than the energy loss due to a collision with the absorber. This enables the absorber integral to be represented as a smooth function of energy. Therefore, the flux is represented by:

$$\Phi(E) = \frac{C(E)}{\left(\sigma_t^A(E) + \sigma_o\right)} \tag{6}$$

2.3 The CENTRM Method

The CENTRM (Continuous ENergy TRansport Module) code solves the Boltzmann transport equation using both point-wise and multigroup cross sections in defined energy ranges, to compute a point-wise flux spectrum. The CENTRM code divides the energy range into three intervals: upper multigroup range, point-wise range, and lower multigroup range. The energy boundaries of these ranges can be controlled by the user. However, it is desirable to set the boundaries of the point-wise energy range such that it includes the resonance structure of an important isotope. This way, a detailed flux calculation in the resonance range can be obtained. Calculations can be performed for an infinite homogeneous medium or for one-dimensional problems having a slab, cylindrical or spherical geometry. Several methods are available for solving the transport equation in the multigroup and point-wise energy ranges. The methods for multigroup calculations are: discrete ordinates (S_N), diffusion, homogenized infinite medium, zone-wise infinite medium, and B_N. For the point-wise calculations, the S_N, collision-probability, homogenized infinite medium and zone-wise infinite medium methods exist.

3. Effect of Bondarenko and Flux Calculator Self-Shielding Methods on ^{238}U Cross Sections

In this paper, we concentrate on the effect of different self-shielding methods on ^{238}U. As shown in Figure 1, ^{238}U has significant resonances especially in the energy range of ~5eV to 10keV. Calculating proper cross sections in the resonance energy range for this isotope is

important for criticality safety problems, particularly for systems containing low-enriched uranium fuel rods. Therefore, as an initial analysis, the Bondarenko and flux calculator methods were used in NJOY to calculate self-shielded cross sections of ^{238}U from ENDF/B-VI. A set of dilution cross sections were used, including: 10^{10} (infinite dilution), 10^6, 10^5, 10^4, 5000, 2500, 1000, 500, 250, 100, 50, 25, 10, and one barn. The flux as a smooth function of energy (C(E) in Equations (4) and(6)) for both methods comprised three functions, including a fission spectrum in the fast energy range, 1/E in the intermediate and thermal Maxwellian in the thermal energy range. The 238-group LAW library [5] group structure was used. In order to compare the effect of the two methods, ratios of group- and dilution-dependent self-shielding factors were calculated. The self-shielding factor for a dilution i in group g ($F_{i,g}$) is defined as the ratio of the total cross-section, for dilution i in group g, to the total cross-section for infinite dilution in group g. The differences in the Bondarenko and flux calculator methods were determined by the ratio of their self-shielding factors:

$$R_{i,g} = \frac{F_{i,g}^{BNDR}}{F_{i,g}^{FLXC}} = \frac{\sigma_{t,i,g}^{BNDR} \Big/ \sigma_{t,\infty,g}^{BNDR}}{\sigma_{t,i,g}^{FLXC} \Big/ \sigma_{t,\infty,g}^{FLXC}} \tag{7}$$

where:

$R_{i,g}$: Ratio of self-shielding factors for dilution i in group g

$F_{i,g}^{BNDR}$, $F_{i,g}^{FLXC}$: Self-shielding factors for dilution i in group g, of the Bondarenko and flux calculator methods, respectively

$\sigma_{t,i,g}^{BNDR}$, $\sigma_{t,i,g}^{FLXC}$: Multigroup total cross-section of dilution i in group g, for the Bondarenko and flux calculator methods, respectively

$\sigma_{t,\infty,g}^{BNDR}$, $\sigma_{t,\infty,g}^{FLXC}$: Multigroup total cross-section at infinite dilution in group g, for the Bondarenko and flux calculator methods, respectively

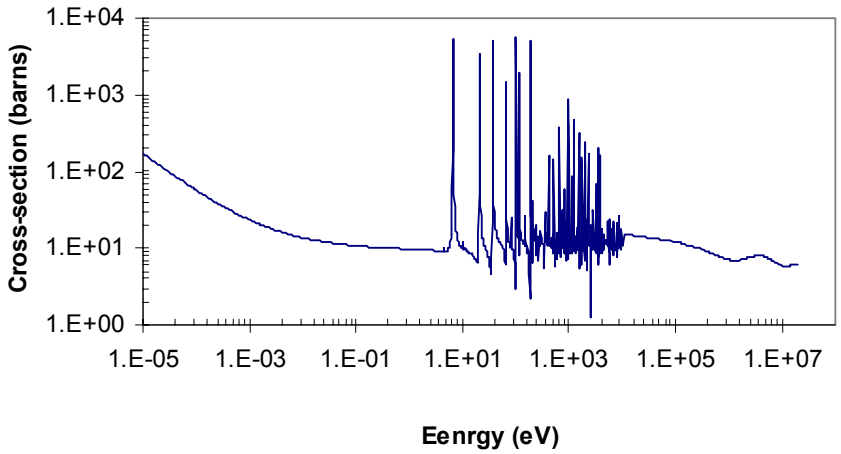

Figure 1 ^{238}U total cross sections.

Figure 2 shows ratios of self-shielding factors calculated by Equation (7), for a dilution of 50 barns. The figure illustrates the significant differences of the two self-shielding methods on cross sections in the resonance energy range.

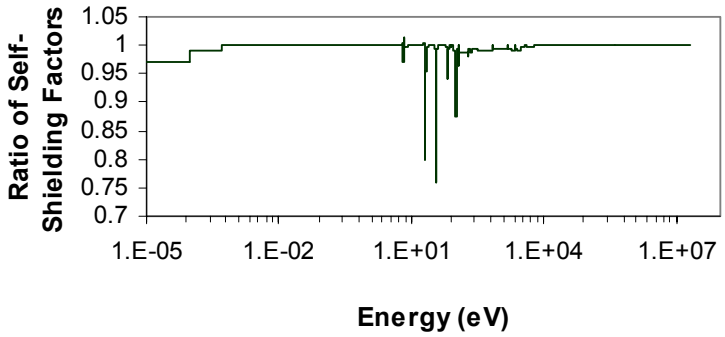

Figure 2 Ratio of Bondarenko to flux calculator self-shielding factors as a function of energy for a dilution cross-section of 50 barns.

Table 1 presents the energy groups that contain the three largest differences in Bondarenko to flux calculator self-shielding factors for thirteen dilution cross sections ranging from $1x10^6$ to one barn. In Table 1, it is observed that the differences in Bondarenko and flux calculator self-shielded cross sections increase as the dilution cross-section decreases. For example, for 50 barns of dilution, the maximum ratio of the self-shielding factors of the two methods is 0.7585 which occurs in the group having boundaries from 35.5 to 37.0eV.

4. Application of Different Self-Shielding Methods on ^{238}U Cross Sections in Criticality Benchmark Cases

The calculations in this section involve the use of the NJOY code (version 99.81) to calculate ^{238}U self-shielded cross sections in an infinite homogeneous medium. ENDF/B-VI data were used for ^{238}U. The Bondarenko, flux calculator and CENTRM methods were used for self-shielding calculations. The 238-group LAW group structure was utilized in NJOY. The new ^{238}U self-shielded cross sections were included in the LAW library using the AJAX module [3]. Note that the cross-sections in the LAW library are based on ENDF/B-V data except six isotopes (^{14}N, ^{15}N, ^{16}O, ^{154}Eu, ^{155}Eu) are from ENDF/B-VI.

The SCALE code package [3] was used with a set of criticality safety analysis sequences. The selected sequences used the BONAMI, NITAWL, and KENO V.a codes. For nuclides in the LAW library other than ^{238}U, the BONAMI code performs self-shielding calculations in the unresolved energy range. For ^{238}U cross-sections calculated by the Bondarenko and flux calculator methods in NJOY, BONAMI performs self-shielding calculations in resolved and unresolved energy ranges. The NITAWL code uses the Nordheim Integral Treatment for self-shielding calculations for the nuclides in the LAW libraries other than ^{238}U. Finally the Monte Carlo criticality code KENO V.a was used to calculate the multiplication factor. Note that the KENO V.a code uses multigroup cross sections.

The Bondarenko and flux calculator methods were used in NJOY by specifying the proper options in the GROUPR module. In order to implement the CENTRM method in NJOY, the CENTRM code was used for a fuel cell in the problem of interest. Evaluations used in the point-wise data were consistent with those in the multigroup data provided to CENTRM. For consistency, data for ^{238}U were taken from ENDF/B-VI. The average scalar flux spectrum in the fuel region was input in the GROUPR module of NJOY in TAB1 format as a weighting function to calculate ^{238}U multigroup cross sections.

Table 1 Ratios of Bondarenko to flux calculator self-shielding factors for groups that show the three largest differences in the two methods

Dilution cross-section (barns)	Ratio of Bondarenko to flux calculator self-shielding factors	Lower Energy (eV)	Upper Energy (eV)
$1x10^6$	0.9996	3.55E+01	3.70E+01
	0.9996	2.00E+01	2.10E+01
	0.9997	1.00E+02	1.08E+02
$1x10^5$	0.9963	3.55E+01	3.70E+01
	0.9966	2.00E+01	2.10E+01
	0.9968	1.00E+02	1.08E+02
$1x10^4$	0.9743	2.00E+01	2.10E+01
	0.9759	3.55E+01	3.70E+01
	0.9762	1.00E+02	1.08E+02
$5x10^3$	0.9582	2.00E+01	2.10E+01
	0.9623	1.00E+02	1.08E+02
	0.9629	3.55E+01	3.70E+01
$2.5x10^3$	0.9365	2.00E+01	2.10E+01
	0.9452	3.55E+01	3.70E+01
	0.9457	1.00E+02	1.08E+02
$1x10^3$	0.9011	2.00E+01	2.10E+01
	0.9122	3.55E+01	3.70E+01
	0.9228	1.00E+02	1.08E+02
500	0.8723	2.00E+01	2.10E+01
	0.8793	3.55E+01	3.70E+01
	0.9072	1.00E+02	1.08E+02
250	0.8421	3.55E+01	3.70E+01
	0.8452	2.00E+01	2.10E+01
	0.8945	1.00E+02	1.08E+02
100	0.7928	3.55E+01	3.70E+01
	0.8160	2.00E+01	2.10E+01
	0.8827	1.00E+02	1.08E+02
50	0.7585	3.55E+01	3.70E+01
	0.8003	2.00E+01	2.10E+01
	0.8756	1.00E+02	1.08E+02
25	0.7261	3.55E+01	3.70E+01
	0.7889	2.00E+01	2.10E+01
	0.8636	1.00E+02	1.08E+02
10	0.6816	3.55E+01	3.70E+01
	0.7769	2.00E+01	2.10E+01
	0.8264	1.00E+02	1.08E+02
1	0.5446	3.55E+01	3.70E+01
	0.6785	1.00E+02	1.08E+02
	0.7390	2.00E+01	2.10E+01

The criticality problem used in this study was selected from the International Handbook of Evaluated Criticality Safety Benchmark Experiments [6]. The problem chosen from the handbook, identified as LEU-COMP-THERM-003, contains water-moderated U(2.35)O_2 fuel rods in 1.684cm square pitched arrays. This benchmark problem contains low enriched Uranium fuel, and has a thermal spectrum. Twenty-three critical configurations (cases) exist for this benchmark problem; cases 1 to 8 contain fuel rods arranged in a single cluster, and cases 9 to 23 contain several cluster configurations. Cases 6, 7 and 8 include water holes, aluminum clad voids, and water filled aluminum tubes, respectively. Cases 1 through 21 contain Gadolinium impurity in water, whereas no Gadolinium impurity exits in cases 22 and 23. This problem was particularly selected due to its low ^{238}U dilution cross sections of ~50 barns within the resonance energy range. The benchmark-model multiplication factor (k-eff) is 1.000 ± 0.0039.

The k-eff calculated in KENO V.a all have less than 0.1% statistical uncertainty. In addition to KENO V.a, continuous energy MCNP [7] calculations were performed to compare with the KENO V.a results. ENDF/B-V data were used in MCNP, except for ^{16}O and ^{238}U; these two nuclides were based on ENDF/B-VI data. Also, k-eff values calculated by MCNP have less than 0.1% of statistical uncertainty. Figures 3, 4 and 5 show k-eff values calculated by KENO V.a using Bondarenko, flux calculator and CENTRM self-shielding methods in ^{238}U, respectively, in comparison to continuous energy MCNP. Multiplication factors calculated using Bondarenko and CENTRM self-shielding methods in ^{238}U are mostly higher relative to the k-eff of MCNP, whereas the k-eff values calculated with multigroup data containing the flux calculator method for ^{238}U are mostly lower relative to the MCNP k-eff values. Table 2 gives the differences of k-eff in pcm (per cent mille) for different self-shielding methods used for ^{238}U in KENO V.a calculations versus those from MCNP. All three self-shielding methods used in KENO V.a have differences less than 500pcm in k-eff, with MCNP.

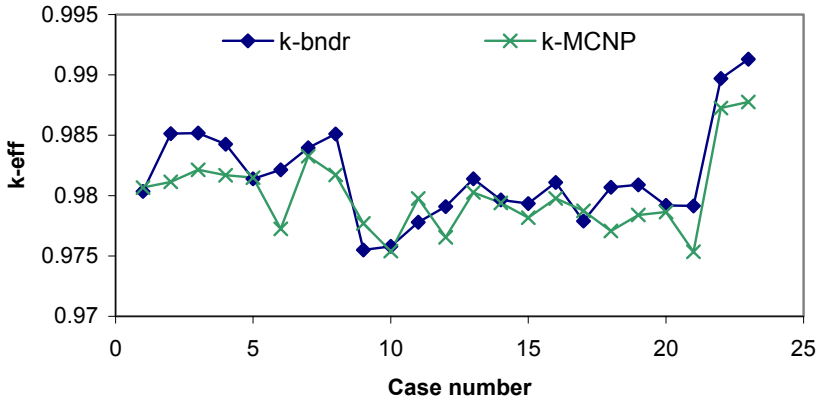

Figure 3 k-eff calculated using the Bondarenko (bndr) self-shielding method for ^{238}U in multigroup KENO V.a and using continuous energy MCNP.

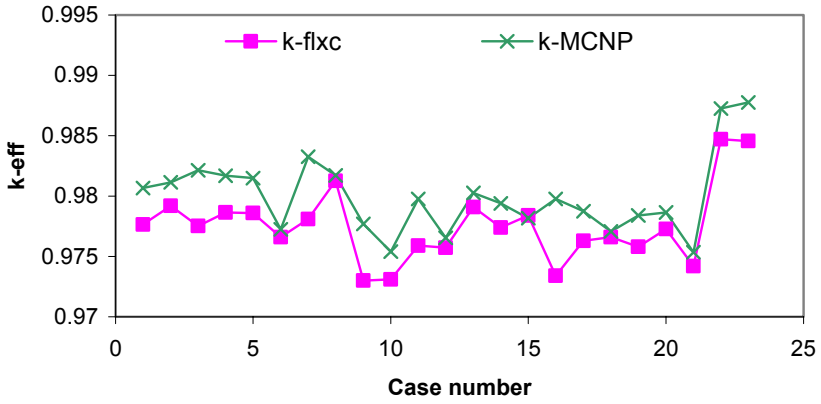

Figure 4 k-eff calculated using the NJOY flux calculator (flxc) self-shielding method for ^{238}U in multigroup KENO V.a and using continuous energy MCNP.

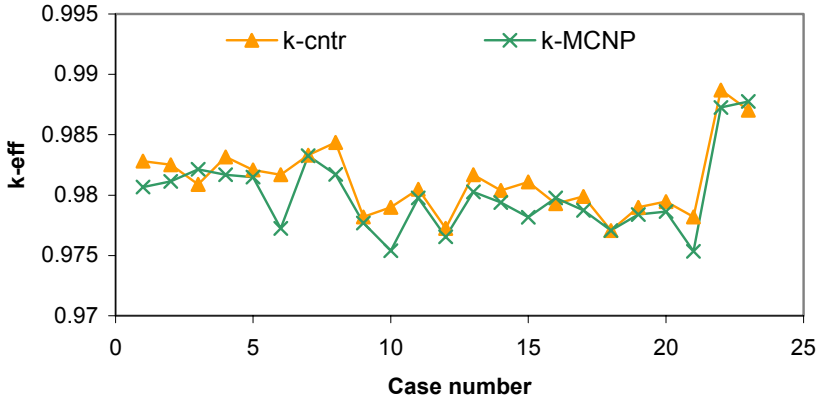

Figure 5 k-eff calculated using the CENTRM (cntr) fluxes in self-shielding of ^{238}U in multigroup KENO V.a and using continuous energy MCNP.

Table 2 Differences in multiplication factors: continuous energy MCNP versus multigroup KENO V.a

Case number	$(k\text{-eff})_{MCNP} - (k\text{-eff})_{KENO\ V.a}$ (pcm)		
	Bondarenko method in KENO V.a	Flux calculator method in KENO	CENTRM method in KENO V.a
1	31	303	-214
2	-399	195	-135
3	-306	462	123
4	-256	306	-145
5	8	288	-62
6	-490	64	-446
7	-72	515	-5
8	-339	45	-264
9	218	468	-52
10	-41	229	-361
11	198	387	-73
12	-256	83	-70
13	-114	117	-144
14	-24	200	-100
15	-116	-21	-293
16	-132	636	46
17	85	245	-115
18	-364	46	0
19	-250	260	-60
20	-56	138	-82
21	-381	114	-286
22	-245	254	-145
23	-354	319	72

5. Conclusions

In this paper the effect of three self-shielding methods for calculating ^{238}U cross sections taken from ENDF/B-VI were analyzed. The three self-shielding methods included the Bondarenko method, flux calculator of NJOY and the CENTRM method. These self-shielded ^{238}U cross sections generated with the LAW group structure were combined with the LAW library to calculate k-eff in twenty-three low-enriched Uranium criticality safety benchmark cases using multigroup KENO V.a. In addition, continuous energy MCNP calculations were performed to compare with the KENO V.a results. It was observed that, some of the self-shielding methods used for ^{238}U showed differences more than 500pcm in k-eff, among themselves for some cases. However, all k-eff values calculated using different self-shielding methods for ^{238}U had differences less than 500pcm with MCNP k-eff. Also, all results were below the benchmark-model k-eff. At ORNL, efforts are currently in progress to develop a new ENDF/B ^{238}U evaluation in support of the DOE NCSP. Further self-shielding analyses will be performed to test the new ^{238}U evaluation and evaluate the performance of the new evaluation relative to the current ENDF/B-VI evaluation.

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