Estimation of the influence of elastic neutron scattering anisotropy on the integral parameters of the model experiment

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Abstract. For the vast majority of isotopes presented in modern evaluated data libraries, the quality of description of elastic neutron scattering anisotropy is difficult to assess due to the lack of critical experiments that are sensitive to these data. This results in a large variation in these data, due to both the difference in the models used in the estimation, and the smoothing of the resonance peculiarities in representation of the energy dependence in the evaluated data files. This work estimates the effect of anisotropy of elastically scattered neutrons based on the model of a critical assembly with a reflector from the tested isotope. Direct estimates of the angular distributions in the evaluated data libraries were compared with the angular distributions, which were reconstructed from the resonance parameters by using Blatt-Biedenharn formula. The thickness of the reflector at which an assembly model became critical is used as a comparison value. The obtained integral characteristics of the elastic scattering anisotropy data, together with the performed comparisons of the detailed dependences of the angular distribution parameters, can serve as a basis for setting tasks to improve the quality of the evaluated data.

1. Introduction

For the vast majority of isotopes presented in modern evaluated data libraries, the quality of description of elastic neutron scattering anisotropy is difficult to assess due to the lack of critical experiments that are sensitive to these data. This results in a large variation in these data, due to both the difference in the models used in the estimation, and the smoothing of the resonance peculiarities in representation of the energy dependence in the evaluated data files.

The purpose of this work is to estimate the quality of the evaluated elastic neutron scattering anisotropy data by comparing the ENDF/B–VIII.0, JEFF-3.3, JENDL-4.0, ROSFOND-2010, BROND-3.1 data libraries using computing parameters of the model of critical assembly. The ICSBEP HEU-MET-FAST-001 (GODIVA) assembly [2] with the radius reduced from 8.7407 cm to 8 cm, surrounded by reflector from mono-isotope under study to achieve criticality, was used as a model assembly. The Dc reflector thickness at which the assembly reaches a critical state was used as an integral characteristic of scattering anisotropy data. The spread of values in the Dc thicknesses obtained as a result of using data from various libraries and various representations of the angular distributions of elastically scattered neutrons is a characteristic of the quality of these data and may serve as a basis for their revision.
The angular distributions of elastic scattered neutrons are kept in the ENDF-6 format [3] in the MF4MT2 sections in form of Legendre polynomial expansion coefficients or $p(\mu)$ tables. For isotopes in which the cross sections in the resonance energy range are represented by resonance parameters (section MF2MT151), there is a possibility of computing the Legendre coefficients in this energy range directly from resonance parameters using the Blatt-Biedenharn formula [4]. So, it gives possibility of additionally check the degree of internal consistency of the data and the adequacy of the representation of the dependence of the angular distribution from energy. The list of isotopes for which the comparison was carried out, was restricted to those for which this possibility is provided in all the libraries under consideration.

To solve the neutron transport task and to calculate the integral characteristics, the MCNP-4c2 program [5] was used with a working library in the ACE format. Preparing the ACE files from the ENDF data libraries, as well as the restoration of angular distributions from the resonance parameters, was carried out by the GRUCON processing software package [6].

2. Calculation results
To compare the effect of anisotropy of elastically scattered neutrons, 15 isotopes were selected in all the libraries under consideration (table 1). As a selection criterion, the value of upper boundary of the resolved resonance range was used: it should be ~ 0.5 MeV in order to cover the region of maximum sensitivity $K_{\text{eff}}$ to the anisotropy of angular distributions in neutron spectrum of the model assembly (near this energy, the spectrum on the surface of the sphere reaches the maximum value).

| Isotope | ENDF/B-VIII.0 | JEFF-3.3 | JENDL-4.0 | ROSFOND-2010 | BROND-3.1 |
|---------|---------------|-----------|-----------|--------------|-----------|
| 011Na023 | 5.000E+5      | 4.593E+5  | 3.500E+5  | 5.000E+5     | 4.593E+5  |
| 012Mg024 | 5.200E+5      | 5.200E+5  | 5.200E+5  | 5.200E+5     | 5.200E+5  |
| 014Si028 | 1.750E+6      | 1.750E+6  | 1.750E+6  | 1.750E+6     | 1.750E+6  |
| 014Si030 | 1.500E+6      | 1.500E+6  | 1.500E+6  | 1.500E+6     | 1.500E+6  |
| 016S_032 | 1.566E+6      | 1.660E+6  | 1.566E+6  | 1.450E+6     | 1.566E+6  |
| 024Cr050 | 7.830E+5      | 7.830E+5  | 6.000E+5  | 7.920E+5     | 7.830E+5  |
| 024Cr052 | 1.430E+6      | 1.430E+6  | 1.430E+6  | 1.200E+6     | 1.200E+6  |
| 024Cr054 | 8.340E+5      | 8.340E+5  | 7.500E+5  | 7.500E+5     | 8.340E+5  |
| 026Fe054 | 1.036E+6      | 7.000E+5  | 7.000E+5  | 7.000E+5     | 7.000E+5  |
| 026Fe056 | 8.500E+5      | 8.500E+5  | 8.500E+5  | 8.500E+5     | 8.500E+5  |
| 028Ni058 | 8.120E+5      | 8.120E+5  | 8.120E+5  | 8.120E+5     | 8.120E+5  |
| 028Ni062 | 6.000E+5      | 6.000E+5  | 5.570E+5  | 6.000E+5     | 6.000E+5  |
| 028Ni064 | 5.530E+5      | 6.000E+5  | 5.530E+5  | 6.000E+5     | 5.530E+5  |
| 082Pb206 | 9.000E+5      | 9.000E+5  | 8.200E+5  | 9.000E+5     | 9.000E+5  |
| 082Pb208 | 1.000E+6      | 1.000E+6  | 1.000E+6  | 1.000E+6     | 1.000E+6  |

The calculations were carried out using the MCNP4c2 code with 1σ statistical error ~ 20 pcm. The set of characteristics were obtained for each isotope of the five reviewed evaluated data libraries, with
angular distributions from the MF4MT2 evaluated data section and reconstructed from resonance parameters. The comparison of obtained results for three isotopes: Na23, Fe56 and Ni58, are presented in the following figures, showing:
1. $K_{\text{eff}}$, as a function of the reflector thickness,
2. $D_c$ critical values of the reflector thickness,
3. $\bar{\mu}$ average cosine as a function of energy.

Figures 1, 8 and 15 shows the dependence of $K_{\text{eff}}$ on the reflector thickness for sodium-23, iron-56 and nickel-58. The vertical dashed lines in the figures of the first type show the minimum and maximum values of the $D_c$ critical thicknesses obtained from the initial data on the angular distributions, the vertical solid lines - those calculated from the resonance parameters (red lines).

Figures 2, 9 and 16 shows the reflector critical thickness for sodium-23, iron-56 and nickel-58 for used libraries. The red (right) columns are for evaluated angular data and the blue (left) are for reconstructed from resonance parameters.

Figures 3-7, 10-14 and 17-21 shows the Legendre Coefficients from ENDF/B-VIII.0, JEFF-3.3, JENDL-4.0, ROSFOND-2010, BROND-3.1 for for sodium-23, iron-56 and nickel-58. The regular line (black) is for MF2MT151 data and the irregular line (red) is for MF4MT2.

2.1 Isotope Na23

![Graph showing Dependence of $K_{\text{eff}}$ on the Na23 reflector thickness](image)

**Figure 1.** Dependence of $K_{\text{eff}}$ on the reflector thickness (Na23).
Figure 2. Na23 reflector’s critical thickness.

Figure 3. Legendre Coefficient from ENDF/B-VIII.0 for Na23.

Figure 4. Legendre Coefficient from JEFF-3.3 for Na23.
Figure 5. Legendre Coefficient from JENDL-4.0 for Na23.

Figure 6. Legendre Coefficient from ROSFOND-2010 for Na23.

Figure 7. Legendre Coefficient from BROND-3.1 for Na23.
2.2 Isotope Fe\textsubscript{56}

![Dependence of $K_{\text{eff}}$ on the Fe\textsubscript{56} reflector thickness](image)

**Figure 8.** Dependence of $K_{\text{eff}}$ on the reflector thickness (Fe\textsubscript{56}).

![Fe\textsubscript{56} reflector's critical thickness](image)

**Figure 9.** Fe\textsubscript{56} reflector's critical thickness.
Figure 10. Legendre Coefficient from ENDF/B-VIII.0 for Fe56.

Figure 11. Legendre Coefficient from JEFF-3.3 for Fe56.

Figure 12. Legendre Coefficient from JENDL-4.0 for Fe56.

Figure 13. Legendre Coefficient from ROSFOND-2010 for Fe56.
2.3 Isotop Ni58

Figure 14. Legendre Coefficient from BROND-3.1 for Fe56.

Figure 15. Dependence of $K_{\text{eff}}$ on the reflector thickness (Ni58).
Figure 16. Ni58 reflector's critical thickness.

Figure 17. Legendre Coefficient from ENDF/B-VIII.0 for Ni58.

Figure 18. Legendre Coefficient from JEFF-3.3 for Ni58.
3. Results discussion

The relative shifts in the values of critical radius of the reflector during the transition of the original files of the estimated file data, in which the parameters of the angular distributions in the resonance region are replaced by those calculated using the Blatt-Biedenharn formula, are given in Table 2. Table 3 gives the integral characteristics averaged over the library: the average critical radius and the relative spread of their values (relative standard deviations) for the initial and calculated angular distributed elastically scattered neutrons.

As can be seen from Table 1, shifts in the values of critical values can have different signs for different isotopes and libraries, caused by a change in the elastic scattering anisotropy when passing from the original data to the calculated ones. With increasing anisotropy (forward scattering probability), the critical radius increases, and vice versa. Some results are quite energy dependent. So, for example, in the case of Na23, the calculated average cosines are obviously higher than those in all libraries, an increase in the critical thickness from ~ 20% to ~ 40% was achieved, which on average is ~ 7 cm (see tables 2, 3).

Indicative at up to -26.73% overshoot for Si30 from the JENDL-4.0 library (table 2), following from a comparison of average cosines. Noteworthy is the fact that the structures listed in the file of the ENDF/B-VIII.0, JEFF-3.0, and BROND-3.1 libraries for this isotope are identical, but the shift of the
resonance feature by ~300 keV with a minus sign with respect to that obtained from the resonance parameters at ~1 MeV. At the same time, good agreement of the initial structure with the calculated one is observed for the Si28 isotope from the same libraries.

In general, this comparison shows that most of the initial data are smoothed in resonance features or are initially smooth as a result of using the optical model. In those cases, when the source file contains data with a high degree of detail (for example, the Cr52 isotope in the ROSFOND-2010 library), replacing the files with those calculated by resonance parameters practically did not affect the result (~0.05%, see Table 1).

For an obvious reason, the identity of the data for the Mg24 isotope in the considered libraries leads to constant increments and zero variance. The critical thicknesses in different libraries are the same when they use the same estimates.

So, for example, Si28 files are the same in JEFF-3.3 and ROSFOND-10, Si30 files are the same in ENDF/B-VIII.0, JEFF-3.3 and BROND-3.1 libraries, S32 files are the same in ENDF/B-VIII.0 libraries, JENDL-4.0 and BROND-3.1, etc.

An interesting fact is that the replacement of the original angular distributions by those reconstructed from the resonance parameters gives, as a rule, a better position between the library, which is manifested in a decrease in the value of the relative standard deviation. This indicates that the estimates of the resonance parameters are in better agreement with each other than the estimates of the angular distributions. An exception is Na23, for which the scatter of the critical thicknesses increased on going to the calculated parameters. A possible explanation is the difference in the formalisms for representing the resonant structure: the library ENDF/B-VIII.0, JENDL-4.0, ROSFOND-2010 use the multilevel Breit-Wigner formula, in JEFF-3.3 and BROND-3.1 - the Reich-Moore formula.

As for the effect of resonance angular distributions on neutron transport and their correlation with the resonance structure of integral cross sections, the task of its study was not set, but preliminary estimates showed that it was negligible even when ~300 groups were used.

Table 2. Relative changes in critical thicknesses in the transition from the original to the calculated parameters of the angular distributions.

| Isotope | ENDF/B-VIII.0 | JEFF-3.3 | JENDL-4.0 | ROSFOND-10 | BROND-3.1 |
|---------|---------------|----------|-----------|------------|-----------|
| Na23    | 38.88%        | 17.95%   | 20.36%    | 40.06%     | 7.78%     |
| Mg24    | 25.74%        | 25.74%   | 25.74%    | 25.74%     | 25.74%    |
| Si28    | 2.28%         | -9.15%   | -0.37%    | 5.84%      | 3.99%     |
| Si30    | 7.44%         | 7.44%    | -26.73%   | -11.39%    | 7.44%     |
| S32     | 7.33%         | 22.69%   | 7.33%     | -0.15%     | 7.33%     |
| Cr50    | -0.79%        | 4.70%    | 2.10%     | 1.64%      | -1.32%    |
| Cr52    | -0.04%        | 3.81%    | 15.17%    | -0.05%     | 0.71%     |
| Cr54    | -3.19%        | 1.94%    | 8.47%     | 7.21%      | -3.54%    |
| Fe54    | -2.57%        | -2.40%   | -5.98%    | -2.40%     | -3.50%    |
| Fe56    | 1.52%         | 0.31%    | 2.41%     | -3.03%     | 4.26%     |
| Ni58    | -9.04%        | 0.10%    | -1.15%    | 0.10%      | 0.33%     |
| Ni62    | 6.88%         | 5.90%    | 3.28%     | 4.66%      | 6.89%     |
| Ni64    | 6.63%         | 6.56%    | 4.72%     | 9.76%      | 6.63%     |
| Pb206   | -2.39%        | -2.64%   | -3.04%    | -2.17%     | -3.93%    |
| Pb208   | -0.48%        | 1.22%    | -0.55%    | -0.62%     | -1.51%    |
### Table 3. Libraries averaged critical thicknesses and relative standard deviations.

| Isotope | Average values of critical thicknesses (cm) | Relative standard deviations |
|---------|-------------------------------------------|-----------------------------|
|         | Initial | Calculated | Initial | Calculated |
| Na23    | 26.23   | 33.15      | 18.1%   | 27.5%      |
| Mg24    | 3.30    | 4.15       | 0%      | 0%         |
| Si28    | 4.91    | 4.92       | 6.7%    | 1.7%       |
| Si30    | 11.48   | 10.85      | 19.1%   | 1.5%       |
| S32     | 26.78   | 28.91      | 17.2%   | 13.2%      |
| Cr50    | 1.58    | 1.60       | 5.9%    | 3.8%       |
| Cr52    | 1.96    | 2.03       | 4.6%    | 4.3%       |
| Cr54    | 1.84    | 1.87       | 13.9%   | 9.0%       |
| Fe54    | 1.48    | 1.43       | 4.2%    | 2.7%       |
| Fe56    | 2.08    | 2.11       | 4.0%    | 2.0%       |
| Ni58    | 1.35    | 1.32       | 3.2%    | 1.2%       |
| Ni62    | 1.31    | 1.38       | 5.2%    | 3.9%       |
| Ni64    | 1.20    | 1.28       | 7.0%    | 5.4%       |
| Pb206   | 2.99    | 2.91       | 1.5%    | 1.4%       |
| Pb208   | 2.73    | 2.72       | 6.4%    | 6.3%       |

### 4. Conclusion

The proposed method for comparing scattering anisotropy based on a criticality calculations of a model assembly with a mono-isotope reflector and using the critical thickness as an anisotropy integral characteristic, makes it possible to assess the degree of agreement between different models and approaches to the description and presentation of the angular distributions of elastically scattered neutrons in the evaluated data libraries.

The Blatt-Biedenharn formula for reconstruction of angular distributions from resonance parameters from, implemented in the GRUCON package, provides an additional check of consistency the integral cross sections with angular distributions, which indicates the possibility of reducing the discrepancies between independent estimates.

The use of angular distributions reconstructed from the resonance parameters leads to a decrease in the scatter of the critical thicknesses of reflectors obtained in calculations based on evaluated angular distributions from different libraries.

The use of angular distributions calculated from the resonance parameters can lead to changes in $K_{eff}$ up to 0.5% for the critical configuration.

Calculations have shown that of all the considered isotopes, nickel is the best reflector. When using a reflector with a thickness of about 1.3 cm, criticality can be achieved while reducing the amount of fissile material by 30%.

The obtained integral characteristics of the elastic scattering anisotropy data, together with the performed comparisons of the detailed dependences of the angular distribution parameters, can serve as a basis for setting tasks to improve the quality of the evaluated data.
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