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**Assessment of the Unresolved Resonance Treatment
for Cross-section and Covariance Representation**

*A report by the Working Party
on International Evaluation Co-operation
of the NEA Nuclear Science Committee*

Co-ordinator

L. Leal
Oak Ridge National Laboratory
United States of America

Monitor

K. Shibata
Japan Atomic Energy Agency
Japan

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The parties to the project are: ENDF (United States), JEFF/EFF (NEA Data Bank member countries) and JENDL (Japan). Co-operation with evaluation projects of non-OECD countries, specifically the Russian BROND and Chinese CENDL projects, are organised through the Nuclear Data Section of the International Atomic Energy Agency (IAEA).

The following report was issued by WPEC Subgroup 32, which investigates the methodologies used in the unresolved resonance region (URR) for cross-section and covariance representation. The objectives of the subgroup were to:

- investigate the use of the Single-level Breit-Wigner formalism in the URR for fissile and fertile isotopes;
- investigate URR parameter representation based on the LSSF = 0 or LSSF = 1 option;
- report on the URR resonance parameter interpolation issue;
- report on the URR covariance representation.

The opinions expressed in this report are those of the authors only and do not necessarily represent the position of any member country or international organisation.

Members of Subgroup 32

L. Leal

Oak Ridge National Laboratory (ORNL), USA

G. Noguère, C. de Saint Jean

Commissariat à l'énergie atomique (CEA Cadarache), France

I. Sirakov

Institute for Nuclear Research and Nuclear Energy (INRNE), Bulgaria

R. Capote

International Atomic Energy Agency (IAEA), Austria

J-C. Sublet

Culham Centre for Fusion Energy (CCFE), United Kingdom

P. Ribon

France

M. Coste-Delclaux, C. Jouanne

Commissariat à l'énergie atomique (CEA Saclay), France

O. Iwamoto, G. Chiba, K. Shibata

Japan Atomic Energy Agency (JAEA), Japan

R.E. MacFarlane, A.C. Kahler, Jr.

Los Alamos National Laboratory (LANL), USA

C.R. Lubitz

Knolls Atomic Power Laboratory (KAPL), USA

D. Cullen

Lawrence Livermore National Laboratory (LLNL), USA

M. Herman

Brookhaven National Laboratory (BNL), USA

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Summary

This report summarises the work performed under WPEC Subgroup 32 (SG32) on issues pertinent to the methodology used in the unresolved resonance region (URR). The main purpose of SG32 was to verify the validity of the Single-level Breit-Wigner (SLBW) cross-section representation in the URR for self-shielding calculations. While SG32 work was under way, several other developments related to the URR on this subject came into play that had a direct impact on the results of calculations.

The work described in this report focuses on:

- testing of the SLBW formalism in the URR for fissile and fertile isotopes;
- URR covariance representation;
- interpolation issue with a URR resonance parameter for the infinitely dilute cross-section calculations;
- ENDF URR parameter representation based on the LSSF = 0 or LSSF = 1 option.

1. Introduction

In the resolved resonance region (RRR), experimental resolution is smaller than the width of the resonances; consequently, resonances can be “seen” and resonance parameters can be extracted via cross-section fitting using methodology such as the R-matrix formalism and generalised least-squares techniques. In the unresolved resonance region (URR), however, fluctuations in the measured cross-sections are smaller than those in the resolved range but are still important for correct calculation of the energy self-shielding of the cross-sections. These fluctuations are due to unresolved multiplets of resonances for which it is not possible to determine parameters of individual resonances as in the resolved region.

The mechanism utilised for cross-section treatment in the unresolved region is based on average values of physics quantities obtained in the resolved range. Average values for level spacing, strength functions, widths and other relevant parameters are used as input for calculations in the URR. Effects such as interference in the fission channels for fissile isotopes, for instance ^{235}U , are very important for self-shielding calculations. These effects are well described with reduced R-matrix formalism, also referred to as Reich-Moore formalism (RM). While the formalism used in the resolved region is adequate to describe the cross-sections, in the URR the cross-sections are represented by the less rigorous Single-level Breit-Wigner (SLBW) formalism. Statistical model codes use the Hauser-Feshbach theory for calculation of average total and partial cross-sections. The energy dependence of the parameters is obtained using various formulations and parameterisation of the level densities, fission barrier penetrations and capture widths. The parameters based on a statistical model analysis of the experimental average cross-sections must then be converted into “equivalent” SLBW parameters in order to be reported in ENDF. The primary use of the average resonance parameters is to reproduce the fluctuations in the cross-sections for the purposes of energy self-shielding calculations.

Subgroup 32 (SG32) was formed to investigate the impact of using SLBW formalism in the URR as it is used in the ENDF. In addition, the ENDF prescription for covariance representation in the URR is also investigated. At the start, the purpose of SG32 was to examine the two issues already mentioned. However, as SG32 activities evolved it became clear that other issues required attention. Therefore SG32 also investigated topics related to the methodology used for generating average resonance parameters in the URR and the conversion to equivalent SLBW parameters, the ENDF

representation for URR parameters based on the LSSF option and interpolation on resonance parameters as opposed to interpolation on cross-sections. Two excellent publications by Sublet [1] and Cullen [2] discuss in detail the impact of using resonance parameter interpolation instead of cross-section interpolation and the use of the LSSF option.

2. URR cross-section self-shielding

The main issue concerning the validity of the URR methodology based on SLBW relies on whether the self-shielding effects on the cross-section are properly calculated. If the cross-section self-shielding effects were unimportant, one would expect the present ENDF methodology to be satisfactory. The URR self-shielding effects were studied for ^{235}U , ^{238}U and ^{239}Pu . These are fissile and fertile isotopes for which the energy level spacing of s-wave resonances is between 0.5 eV and 25 eV, providing the grounds for testing the unresolved resonance formalism. To test whether SLBW formalism is adequate for URR self-shielding calculations, a special ladder code based on NJOY methods was written. This code generates a single “realistic” ladder of resonances based on the statistics of the unresolved resonance range in SLBW, MLBW or RM format and computes cross-sections and self-shielding factors. The results of the impact of SLBW, MLBW and RM in describing the average cross-section and consequently the self-shielding effect are presented.

2.1 Averaged and self-shielded cross-section for ^{235}U

The resonance energy regions for ^{235}U are from 10^{-5} eV to 2.25 keV for the RRR and from 2 250 eV to 25 keV for the URR. The ladder code, with RM formalism in the URR, was used to calculate the elastic scattering, fission and capture cross-sections [3]. The calculations were made with 45 energy groups having widths of 500 eV, with the exception of the first group, which had a width of 750 eV. The results are shown in Figures 1-3.

As can be seen, the percent difference in the infinitely dilute cross-section can be as high as 10%. Although there are differences in the average cross-section, one needs to verify the impact of the SLBW and the RM formalisms in the self-shielded cross-section. The cross-section self-shielding calculations done with the ladder code for a dilution of 10 barns are shown in Figures 4-6.

The self-shielding calculations displayed in Figures 4-6 reveal that the SLBW and RM results are very similar. These results suggest that, for ^{235}U , SLBW formalism in the URR is adequate for describing the self-shielded cross-section. Furthermore, the self-shielding effect in the cross-section in the URR, for ^{235}U , is not very important.

Figure 1: Comparison of the average elastic scattering cross-section for ^{235}U in the URR calculated with the SLBW and RM formalisms

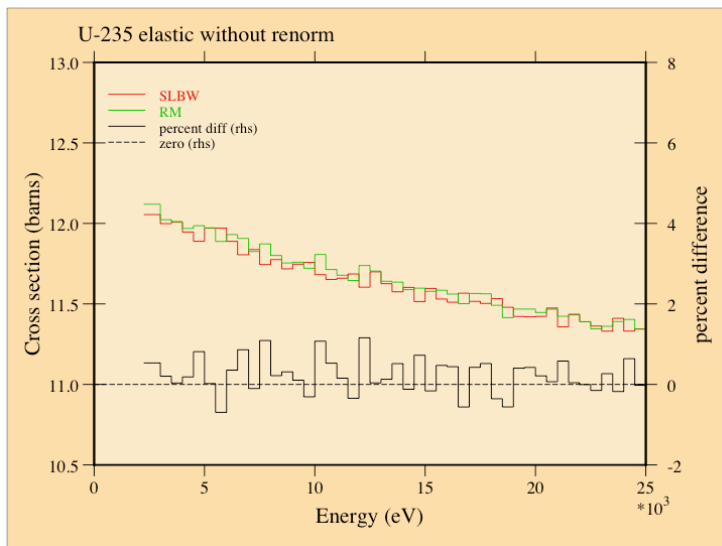


Figure 2: Comparison of the average fission cross-section for ^{235}U in the URR calculated with the SLBW and RM formalisms

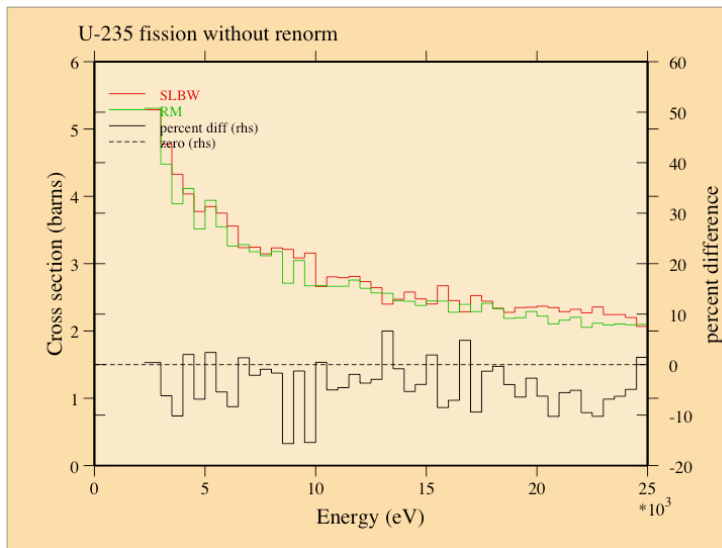


Figure 3: Comparison of the average capture cross-section for ^{235}U in the URR calculated with the SLBW and RM formalisms

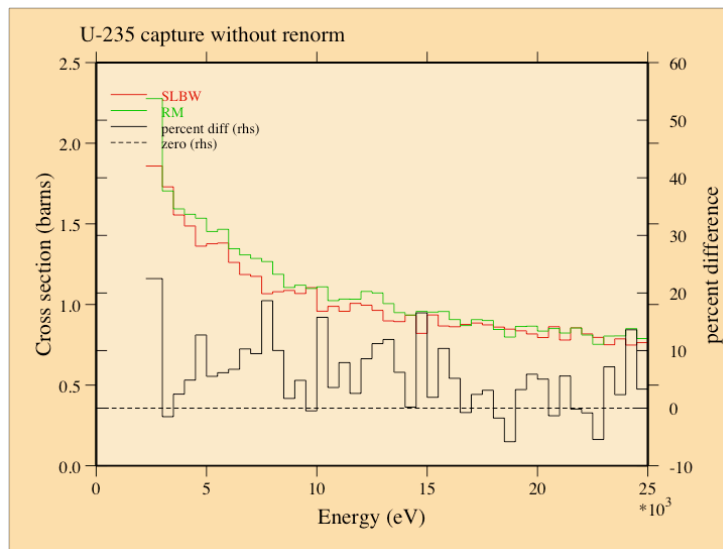


Figure 4: Comparison of the elastic self-shielding factor for ^{235}U in the URR calculated with the SLBW and RM formalisms

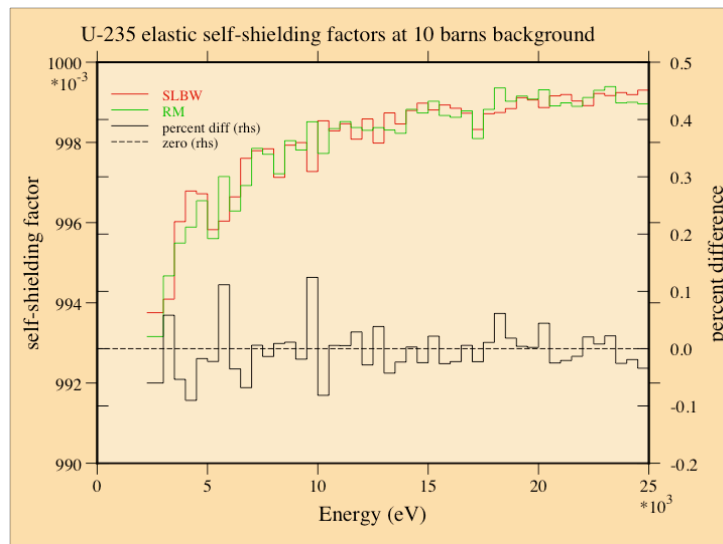


Figure 5: Comparison of the fission self-shielding factor for ^{235}U in the URR calculated with the SLBW and RM formalisms

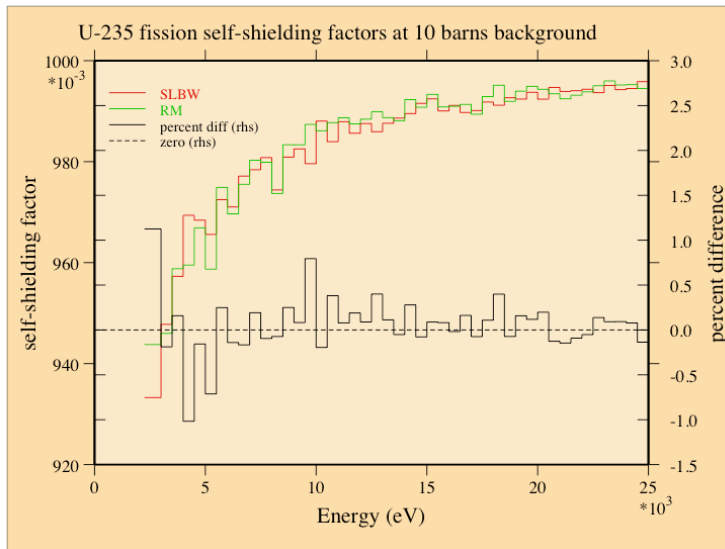
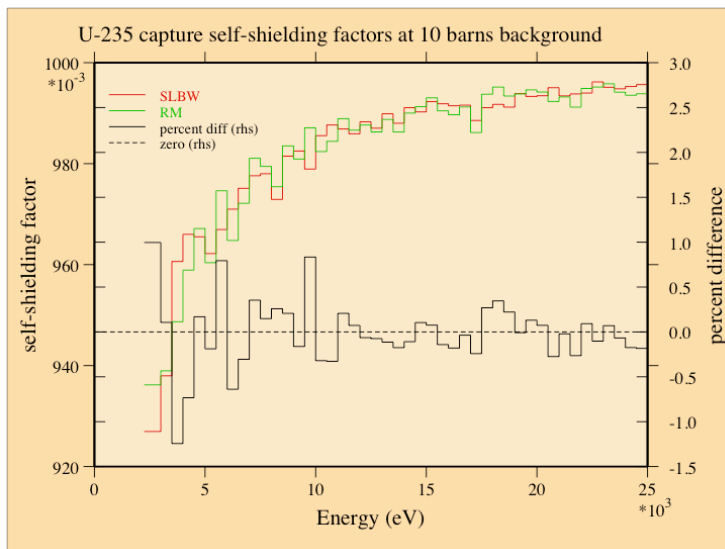


Figure 6: Comparison of the capture self-shielding factor for ^{235}U in the URR calculated with the SLBW and RM formalisms



2.2 Averaged and self-shielded cross-section for ^{238}U

The URR for ^{238}U in the ENDF/B-VII evaluation is from 20 keV to 150 keV. The ladder code, with RM formalism in the URR, was used to calculate the elastic scattering and capture cross-sections. The calculations of dilute elastic and capture cross-sections without normalisation to the smooth FILE 3 cross-sections are shown in Figures 7 and 8, respectively. These are comparisons for the SLBW, MLBW and RM formalisms below the inelastic threshold. The graphs indicate a small decrease in both MLBW and RM elastic cross-sections from the SLBW result. It is found that only a small part of this decrease is due to truncating the negative cross-sections during reconstruction. The difference between MLBW and RM is small for the elastic. For the energy group width used here, there are about 100 s-wave resonances in a group, and assuming a $1/\sqrt{N}$ variation, one expects about 10% fluctuation for one ladder. The results would look smoother with larger groups, and computed reaction rates would also show smaller statistical differences. The capture cross-section is the same for all three methods. The FILE 3 cross-section is also shown.

Figures 9 and 10 show the self-shielding factors for a background cross-section of 1 barn for the elastic cross-section and 10 barns for the capture cross-section. This represents the uncertainties that will be seen in the effective cross-sections after LSSF = 1 renormalisation (discussed in Chapter 5). The fluctuations in the self-shielding factors are smaller than those in the dilute cross-sections. This feature helps to make LSSF = 1 a useful representation in the URR. Differences in the capture for the three methods come from the effect of the total cross-section on self-shielding. The impact of these differences in a benchmark calculation was investigated for the BIGTEN benchmark system. The difference in the effective multiplication factor (k_{eff}) arising from the study with the self-shielding effect being completely neglected was about 0.35%. One can therefore roughly estimate that 30% accuracy in the self-shielded cross-sections would reduce the uncertainty in BIGTEN to 0.1%. The differences in the plot amounting to 0.5% or so would probably be barely visible in Monte Carlo results for BIGTEN. The graphs suggest that for ^{238}U , the use of RM is not preferable to the use of MLBW. SLBW would probably be adequate for such applications as well.

Figure 7: Comparison of the average elastic cross-section for ^{238}U in the URR calculated with the SLBW, MLBW and RM formalisms

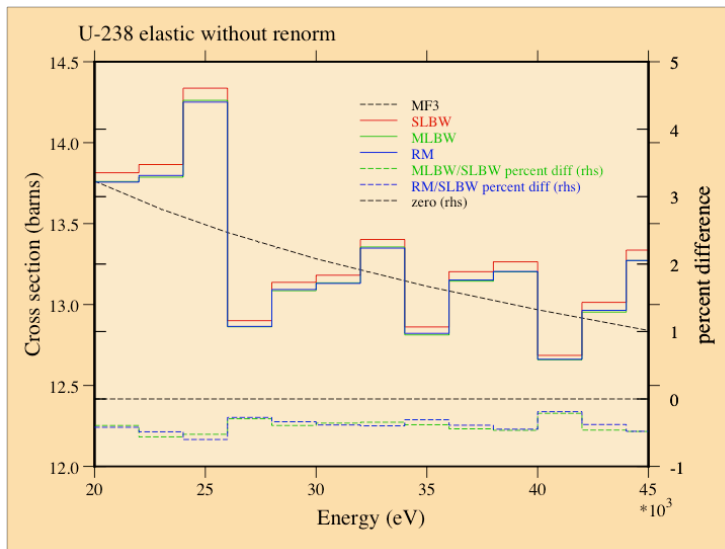


Figure 8: Comparison of the average capture cross-section for ^{238}U in the URR calculated with the SLBW, MLBW and RM formalisms

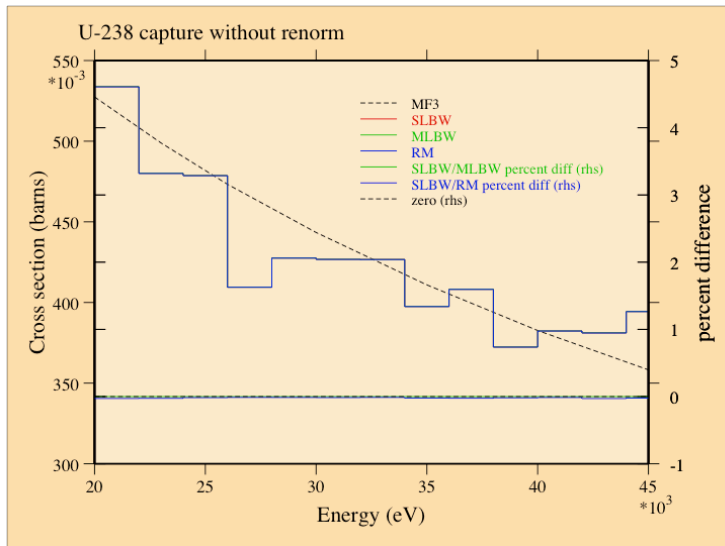


Figure 9: Comparison of the elastic self-shielding factor for ^{238}U in the URR calculated with the SLBW, MLBW and RM formalisms

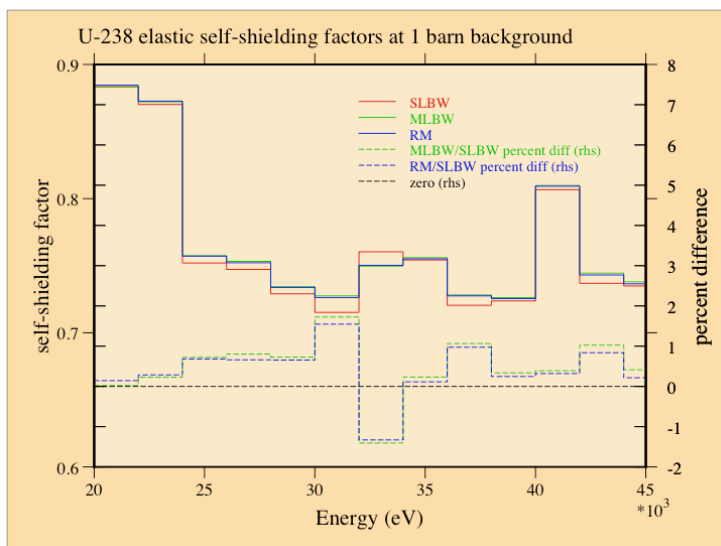
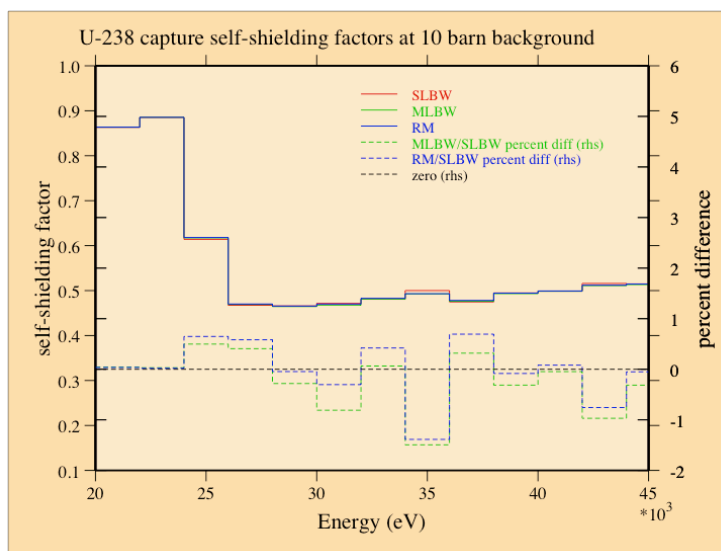


Figure 10: Comparison of the capture self-shielding factor for ^{238}U in the URR calculated with the SLBW, MLBW and RM formalisms



2.3 Averaged and self-shielded cross-section for ^{239}Pu

The URR for ^{239}Pu ranges from 2.5-30 keV. Cross-section and self-shielding factors were calculated using the SLBW, MLBW and RM formalisms in the URR. The cross-sections calculated are the elastic scattering, fission and capture cross-sections. The results are displayed in Figures 11-13. The elastic cross-section results calculated with the SLBW and MLBW formalisms are very similar, whereas the fission and capture results are the same for SLBW and MLBW. The RM results show some apparent differences. The difference can be understood from the fact that additional random numbers are required to generate the two fission channels, which means that the resonance features from RM do not line up with those from SLBW. Therefore, it can be said that the differences are in fact similar to those one would obtain from comparing two statistically independent ladders. With MLBW formalism, the features do line up, and the fluctuations appear to be smaller. When the SLBW result is high, so is the MLBW, and the per cent difference is small.

Figures 14-16 show the self-shielding factors for a background cross-section of 10 barns, which is much lower than one encounters in practical application. The same issues of large fluctuations in the RM formalism are also seen here. The differences between the MLBW and the SLBW formalisms are small.

Figure 11: Comparison of the average elastic scattering cross-section for ^{239}Pu in the URR calculated with the SLBW, MLBW and RM formalisms

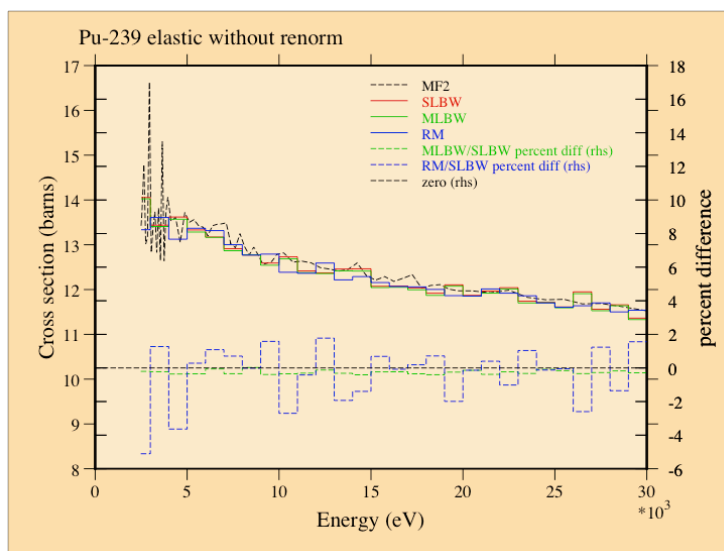


Figure 12: Comparison of the average fission cross-section for ^{239}Pu in the URR calculated with the SLBW, MLBW and RM formalisms

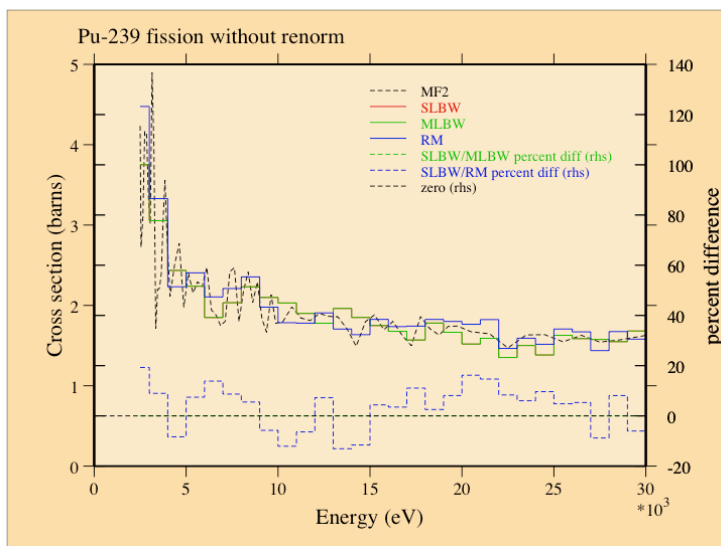


Figure 13: Comparison of the average capture cross-section for ^{239}Pu in the URR calculated with the SLBW, MLBW and RM formalisms

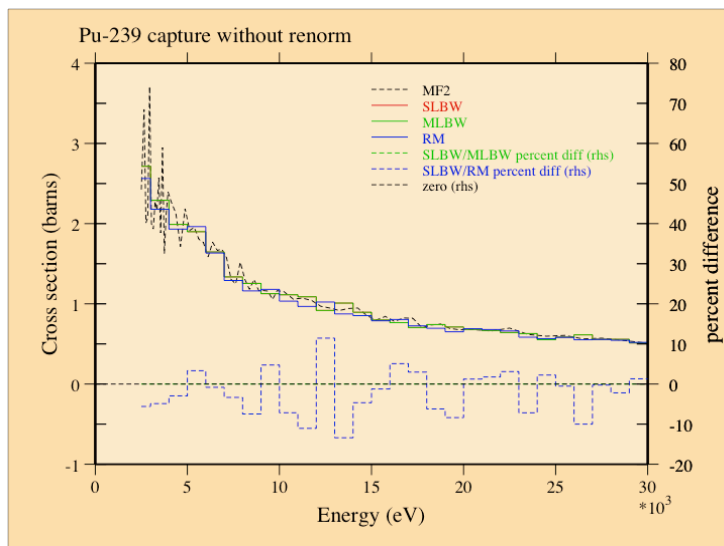


Figure 14: Comparison of the elastic self-shielding factor for ^{239}Pu in the URR calculated with the SLBW, MLBW and RM formalisms

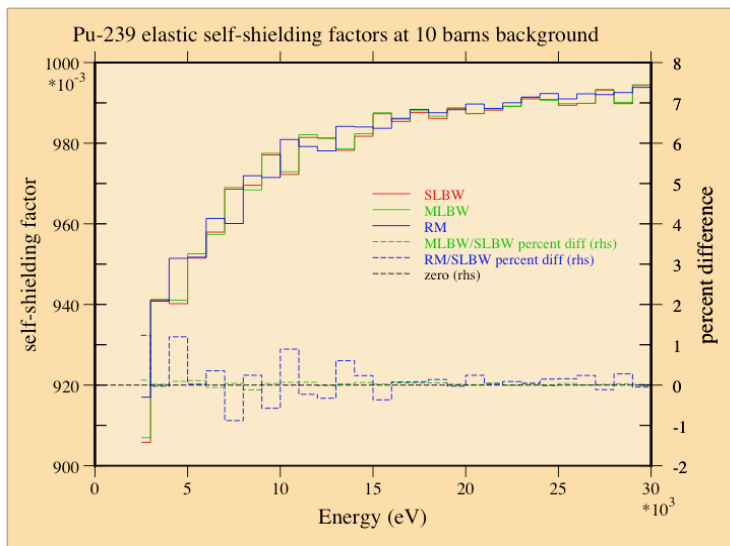


Figure 15: Comparison of the fission self-shielding factor for ^{239}Pu in the URR calculated with the SLBW, MLBW and RM formalisms

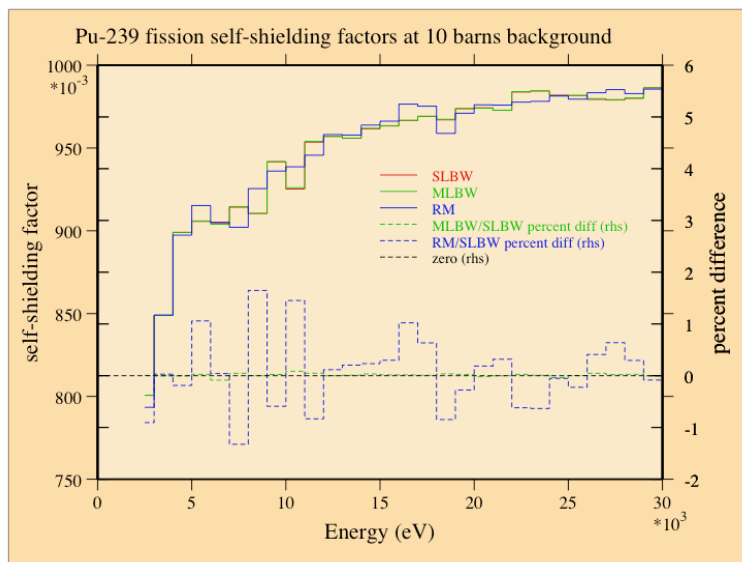
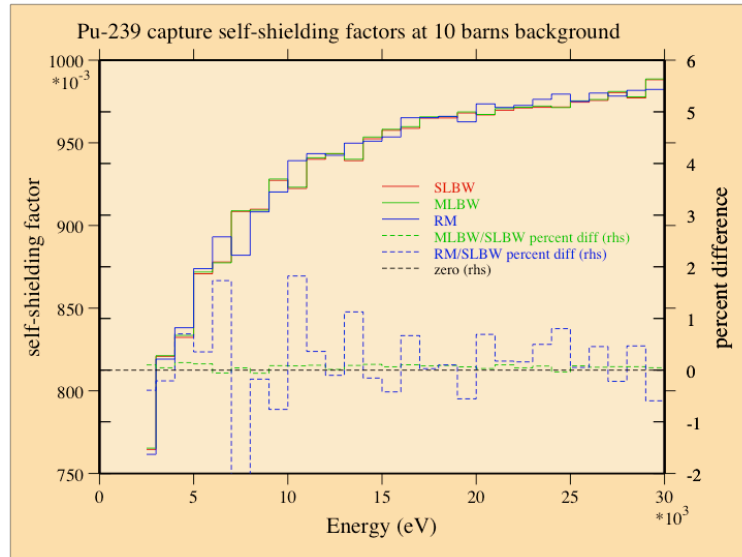


Figure 16: Comparison of the capture self-shielding factor for ^{239}Pu in the URR calculated with the SLBW, MLBW and RM formalisms



Some comments on statistical sampling of resonance parameters follow. Assuming that the scale of fluctuations is $1/\sqrt{N}$, the energy group must be sufficiently wide to have “enough” resonances for sampling. For s-wave resonances with 10 eV average level spacing, the use of 5 keV groups would reduce fluctuations to the 5% level. Of course, a reaction rate averages over the whole range. If fluctuations are balanced around an average value, one can achieve a reasonable reaction rate even with large fluctuations. For the ^{239}Pu URR evaluation, a sharp unphysical change in the average resonance parameters exists at the lower part of the URR (as seen in the FILE 2 parameter). The methods used to compute cross-sections from FILE 2 implicitly assume that the parameters vary slowly with energy over a range that contains many resonances. Therefore, the sharp change in ^{239}Pu violates this rule and can be the source of a problem. Hence, the meanings of the parameters, cross-sections and self-shielding factors at the lower energies are not clear. A re-evaluation of the URR ^{239}Pu resonance parameters is suggested.

3. URR covariance representation

Two issues about the resonance parameter covariance representation in the URR need to be addressed: i) uncertainty in the nuclear radius; ii) energy dependence of the uncertainties in the URR. The current ENDF-6 format does not include a provision for including uncertainty in the nuclear radius. Lack of information on the nuclear radius indicates that the uncertainties in the averaged cross-sections in the URR are small, as discussed by Kawano and Shibata [4]. In addition, a correlation between uncertainty in the nuclear radius and average resonance parameters is needed to achieve a more realistic estimation of the uncertainty in the average cross-section.

The second issue is the energy dependence of the uncertainties in the URR. While the energy dependence of the average resonance parameters in the ENDF-6 [5] can be explicitly used, the covariance representation is energy independent. It appears that some minor change in the processing codes would be required to allow energy dependence of the uncertainty in the URR. These two issues require minor modifications to the current ENDF-6 format.

4. URR resonance parameter interpolation issue

Differences in the infinitely dilute cross-section calculated with the NJOY [6] and the PREPRO [7] codes uncovered an inconsistency in the interpretation of the way interpolation should be performed. The issue arises when using the energy dependence of the average URR parameters (LRF=2). In the LRF=2 option, the URR average resonance parameters are provided by the evaluator on an energy grid, together with an interpolation scheme indicated by the variable INT. The current ENDF procedures indicate that one should compute the unresolved cross-sections at these energy grid points. However, intermediate values are to be obtained by interpolating on the cross-sections using the scheme defined by INT. This approach has the advantage of being economical in the UR calculation and of giving a unique result for the cross-sections. However, the cross-sections that it produces have discrete segments that show up as straight unphysical lines when plotted according to INT. The differences between NJOY and PREPRO results were traced to the way the codes' interpolations were carried out. At the energies where parameters are tabulated, PREPRO and NJOY results agree (i.e. given a unique set of parameters at any given energy, both codes use the same model to calculate cross-sections at that energy). Where they differ is in the interpolation scheme used between the energies at which the average URR parameters are tabulated. NJOY interpolates on cross-sections, whereas PREPRO interpolates on the average URR parameters. A quick read of the ENDF-102 formats and procedures manual indicates that one should interpolate on cross-sections; however, this procedure leads to non-physical results, if the energy steps in the evaluation are too large for the specified cross-section interpolation scheme. After reviewing the details of ENDF-102, it was decided to update NJOY to interpolate on parameters. This action taken, the NJOY and PREPRO results in the URR closely agree. The tolerance for adding additional energy points in large energy intervals using parameter interpolation in NJOY has been tightened up to improve the agreement between NJOY and PREPRO. Similar improvement can be obtained by simply using log-log interpolation in evaluations.

5. URR representation based on the LSSF = 0 or LSSF = 1 option

The FILE 3 cross-sections in the URR are interpreted depending on the flag LSSF. FILE 3 may be regarded as a partial background cross-section (LSSF = 0) to be added to the FILE 2 contributions in order to obtain the infinitely dilute cross-sections. It can also be regarded as the entire diluted cross-section (LSSF = 1), in which case FILE 2 is used exclusively for self-shielding calculations. The motivation for using the LSSF = 1 option comes from the fact that users were noting differences in infinitely dilute cross-sections calculated in the URR. Therefore, the LSSF = 1 option was designed to allow evaluators to include the tabulated infinitely dilute cross-sections in their evaluation, in FILE 3. The convention would then be to use the evaluator's supplied tabulated cross-sections (FILE 3) and the URR parameters (FILE 2) for calculation of the self-shielding factors. It is expected that in the LSSF = 1 option, the infinitely dilute cross-sections calculated from the average resonance parameters are in agreement with those listed in FILE 3. However, this is not the case. Sirakov, *et al.* [8] pointed out that the differences come from the lack of compatibility between the evaluation models – for instance, the use of an optical model for extracting average parameters, and the conversion of these parameters into an equivalent SLBW representation of ENDF. As an example, it can be shown from a link to the optical model that the ENDF SLBW representations misrepresent the shape elastic cross-section, and consequently the total cross-section, by assuming the validity of the first order of approximation in terms of the transmission coefficient T_c (i.e. $\sqrt{1 - T_c} \approx 1 - T_c/2$). In addition, a few other weaknesses exist, such as the fact that the ENDF model assumes no orbital dependence of the scattering radius and also the lack of use of the Moldauer prescription [9] for determining fluctuation factors, etc. If the average cross-sections calculated with the URR parameter were fully compatible with that of FILE 3, the LSSF = 0 option would be recommended. However, until the compatibility issues concerning FILE 2 and FILE 3 are fully understood and addressed, the LSSF = 1 option would be more appropriate.

6. Conclusion

Several issues concerning URR representation are discussed in this report. SG32 intended to examine whether the SLBW representation of the cross-section in the URR was adequate for self-shielding calculations. This task was achieved. However, as SG32 activities evolved, it became clear that other issues required attention. SG32 thus also investigated subjects related to the methodology used for generating average resonance parameters in the URR and the conversion to equivalent SLBW parameters, the ENDF representation of URR parameters based on the LSSF option, and interpolation on resonance parameters as opposed to interpolation on cross-sections. Overall, this report demonstrates that the results using SLBW are appropriate for the URR. It also indicates that interpolation on parameters other than cross-section is advised. Additionally, the LSSF = 1 option should be used.

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