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On the Self-Shielding in the Unresolved Resonance Range

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ABSTRACT

Nuclear reaction cross sections exhibit resonance behaviour. As incident energy increases, the resonance density increases to the point that individual resonances cannot be resolved, but they still contribute to self-shielding. In this energy region resonances are represented by statistical average parameters and methods are described in standard text-books to account for self-shielding by applying some approximations. In Monte Carlo transport methods self-shielding is treated by probability tables or multi-band parameters. The procedures for generating probability tables (or multi-band parameters) for Monte Carlo calculations was questioned. The IAEA organised an exercise to validate codes and methods for generating parameters to describe self-shielding in the unresolved resonance range in Monte Carlo transport calculations.

1 INTRODUCTION

Nuclear reaction cross sections have energy-dependent behavior, where the cross section can change by several orders of magnitude over narrow energy intervals – these are called resonances. The relative resonance density increases with energy to the point, where they cannot be resolved experimentally, but the fluctuations in the cross sections still contribute to the so-called self-shielding effect. Self-shielding occurs because resonances deplete neutrons near the resonance energies, thus effectively reducing reaction rates. Standard text-books on reactor physics address the self-shielding effect in the unresolved resonance range using various approximations by defining average resonance parameters, which are then used to derive self-shielded cross sections. An alternative method usually applied in Monte Carlo transport codes is to define probability tables or multi-band parameters to tackle self-shielding.

An exercise was performed at the International Atomic Energy Agency (IAEA) to validate methods of processing nuclear data to make application libraries in the so-called ACE format for use in various Monte Carlo transport codes [1]. Probability tables give the probabilities that in a certain energy interval the cross section lies within a certain range of cross section values. About 20 bins are commonly used in the libraries in ACE format available from the Los Alamos National Laboratory (LANL). They are usually prepared by generating resonance ladders by statistically sampling resonances from the unresolved resonance parameters and averaging the cross sections from the ladders. Alternatively, multi-band parameters are derived by the conservation of moments. Two bands are usually sufficient. The method of generating multi-band parameters is described in detail in an IAEA publication available on the web [2]. Previous exercise has demonstrated that multi-band parameters and probability tables can be used interchangeably [3].

In an effort to provide to the IAEA Member States an independent route to generating application libraries, a project was initiated that produced the ACEMAKER code [4], which is a module for assembling partly processed data using the PREPRO package [5]. The GROUPIE module of package version PREPRO2019 has been reorganized to simplify the processing.

The main objectives of this paper are: (i) to test the impact of Unresolved Resonance Region (URR) self-shielding, (ii) compare the results based on a variety of URR self-shielding models, (iii) define the problems we see with URR self-shielding models to encourage future work to solve this problem.

2 TEST EXAMPLE

The test problem is a simple sphere of 1 m radius made of ^{139}La with a mono-energetic isotropic neutron source of 20 MeV. The source at this energy produces a conveniently high neutron flux at energies that are important for self-shielding. The ^{139}La data are taken from the ENDF/B-VIII.0 library [6]. This element was chosen because it is mono-isotopic and its unresolved resonance parameters seem to have inconsistencies that will be emphasized in this paper. Furthermore, ^{139}La is one of the less important materials and many evaluated data libraries basically adopt more or less the same data with minimal changes.

The observable in this exercise is the leakage spectrum from the surface of the sphere. For convenience the TART 616-group structure was chosen to display the results because it is one of the standard group structures in PREPRO. The groups are equidistant in lethargy, hence the group flux is equal to the lethargy spectrum.

3 CROSS SECTIONS AT INFINITE DILUTION

The main cross sections of ^{139}La are shown in Figure 1. The fine-group total cross section plot in the unresolved resonance range (20 keV – 100 keV) in Figure 2 shows the discontinuity in the cross sections at the resolved/unresolved resonance boundary at 20 keV.

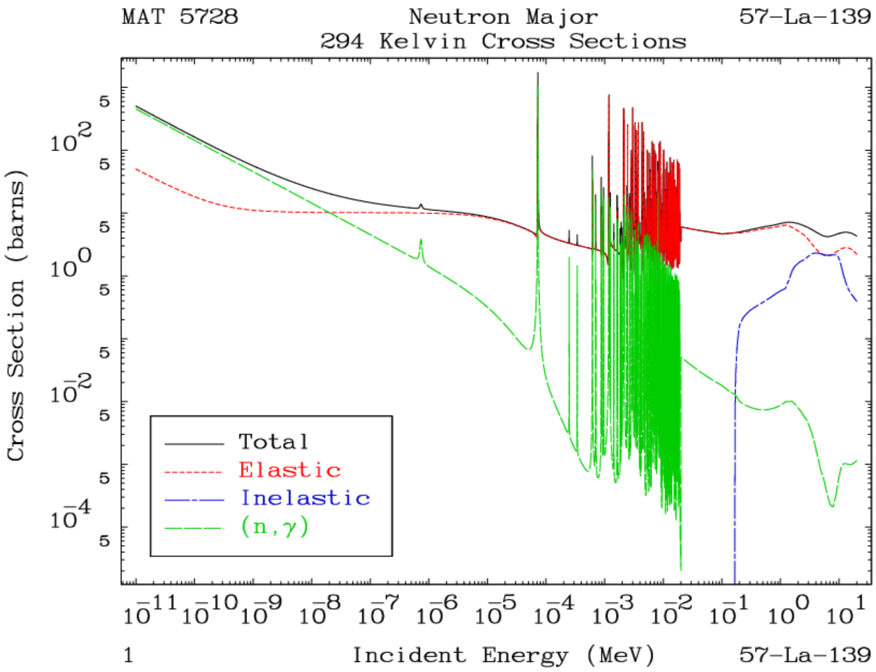

Figure 1: The main cross sections of ^{139}La from the ENDF/B-VIII.0 library.

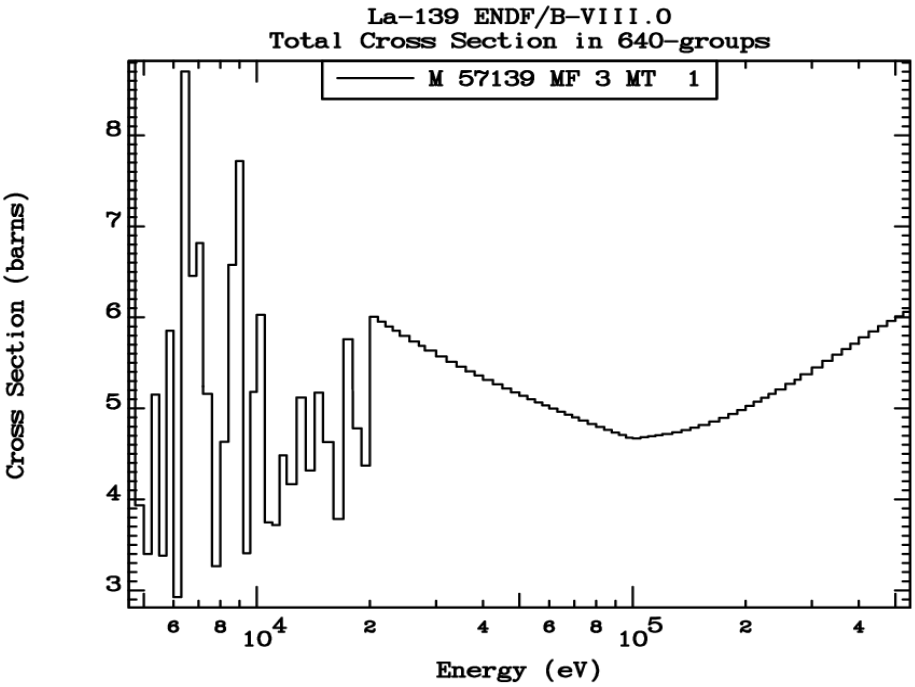

Figure 2: The fine-group total cross section of ^{139}La in the unresolved resonance range.

4 CALCULATED NEUTRON LEAKAGE SPECTRA

Leakage spectra were calculated with the MCNP continuous-energy Monte Carlo transport code using ACE data files prepared in different ways. Cross section processing and final ACE file assembly were done with NJOY2012. Probability tables were calculated with the PURR module of NJOY, while all multi-band parameters were calculated with the local URRDO153 code based on the self-shielded cross sections generated by the UNRESR or PURR modules of NJOY. Alternatively, the multi-band parameters generated by the GROUPIE module of PREPRO were used. The “fully-shielded” cases correspond to the Bondarenko dilution cross section of zero barns.

4.1 The impact of self-shielding

Figure 3 shows the importance of self-shielding in the test problem. Without URR self-shielding (red) there is a strong discontinuity in the calculated spectrum at the top of the resolved resonance region (RRR) (i.e. 20 keV), which can be attributed to the discontinuity in the cross sections, shown in Figure 2. There is no discontinuity at the upper end of the URR (100 keV), since the cross sections are continuous.

Fully-shielded cross sections (blue) produce a spectrum very close to the one with cross sections at nominal self-shielding with probability tables (black), which is to be expected due to the large bulk of the material.

The spectrum at the upper end of URR (100 keV) with shielded cross sections shows very large discontinuity, which implies a very strong self-shielding effect at this energy. Considering our knowledge of the resonance structure of similar nuclei at these energies, such strong self-shielding seems to be clearly unphysical.

At lower energies (down to 20 keV) there is interference between slowing-down and self-shielding. The calculated spectra with shielded and unshielded cross sections are virtually the same due to cancellation of errors.

4.2 Comparison of spectra using different methods for self-shielding treatment

The calculated leakage spectra with probability tables or multi-band parameters produced in different ways are shown in Figure 4.

The spectrum calculated with probability tables from the PURR module (red) is practically equal to the spectrum calculated with two-band parameters derived from the probability tables (blue). This equivalence has already been discussed in previous work, documented in INDC(NDS)-0701 [3]

The spectrum calculated with two-band parameters derived from the self-shielded cross sections calculated by the UNRESR module of NJOY (green) shows a similar trend, but with a considerably smaller discontinuity at 100 keV.

The spectrum calculated with multi-band parameters from PREPRO (black) does not have a non-physical discontinuity at the upper end of the URR (100 keV). The bump at the lower end (20 keV) is due to the discontinuity in the cross sections at infinite dilution.

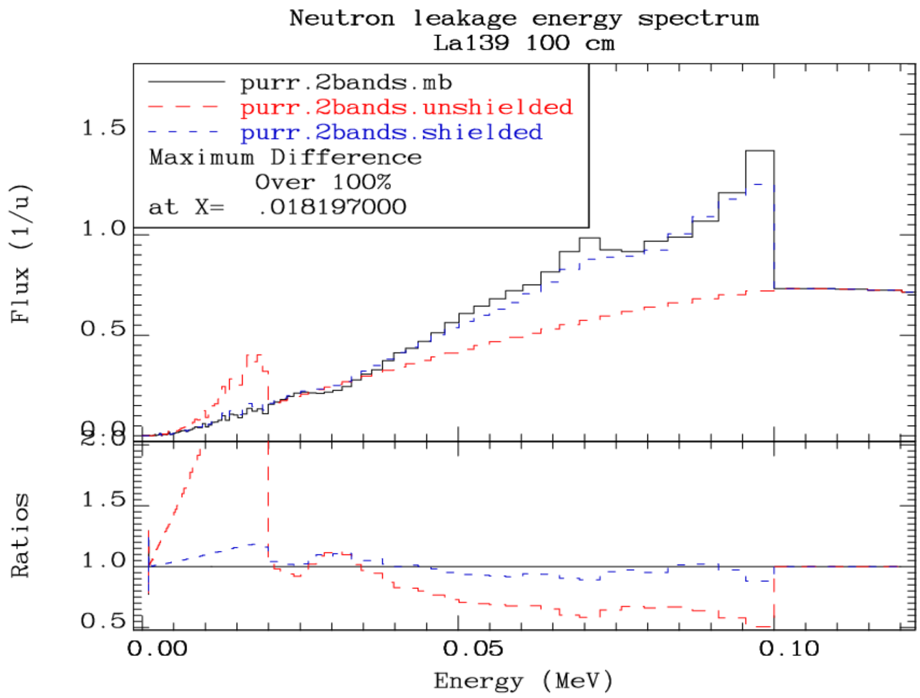

Figure 3: Leakage spectra in URR calculated with and without self-shielding

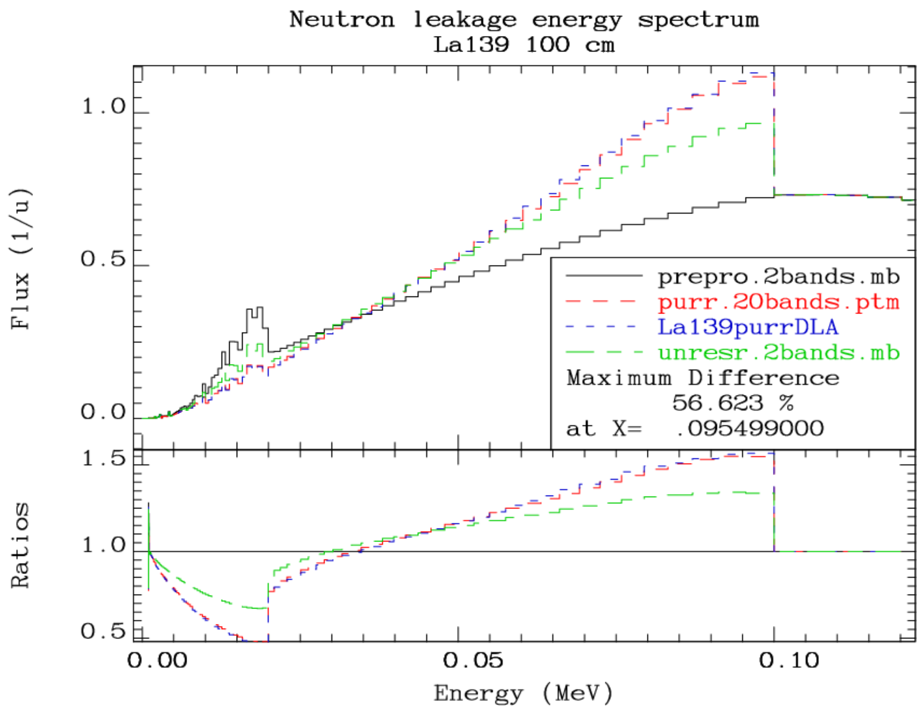

Figure 4: Leakage spectra in URR calculated with different methods of generating probability tables or multi-band parameters.

4.3 Comparison self-shielded cross sections

The self-shielded cross sections as a function of the Bondarenko dilution cross section differ significantly. The cross sections for incident neutrons of 20 keV are shown in Figure 5, and at 100 keV in Figure 6. At 0.1 barn dilution cross section the values of self-shielded cross sections are as follows:

- At 20 keV the method of PREPRO gives cross section value that is 19 % smaller and the PURR method gives value that is 40 % smaller than at infinite dilution.
- At 100 keV the PREPRO value is only 4 % smaller and the PURR value is still 20 % smaller than at infinite dilution

The differences in the cross sections explain the differences in the calculated leakage spectra. It should be pointed out that such strong self-shielding as given by PURR is physically unreasonable.

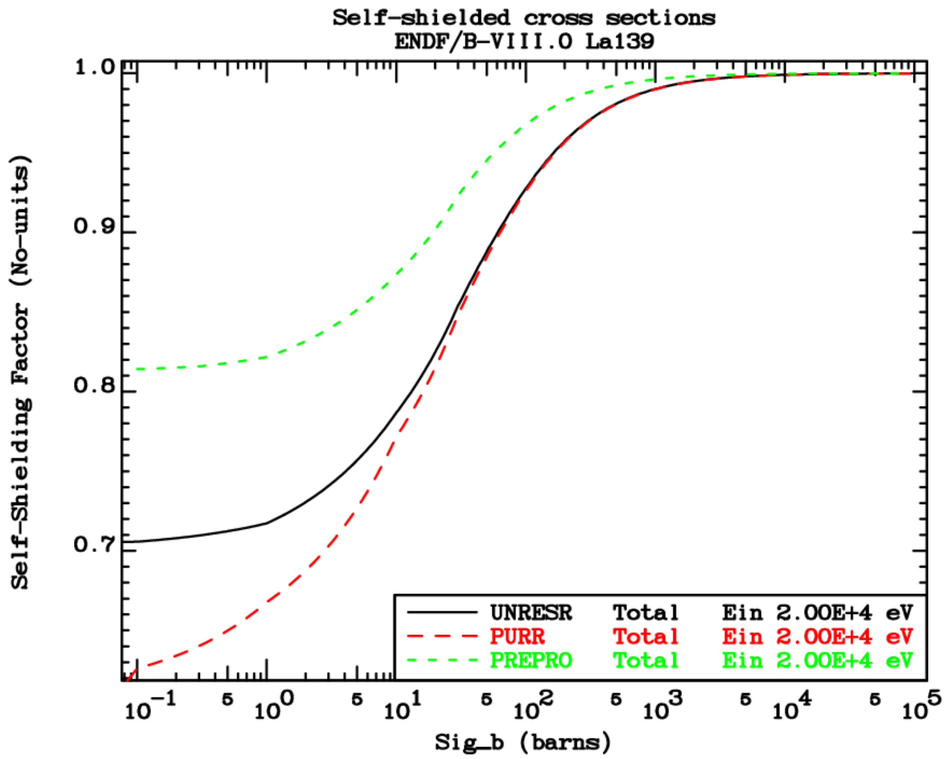

Figure 5: Self-shielded cross sections as a function of the Bondarenko dilution cross section for incident neutrons of 20 keV, produced by different methods.

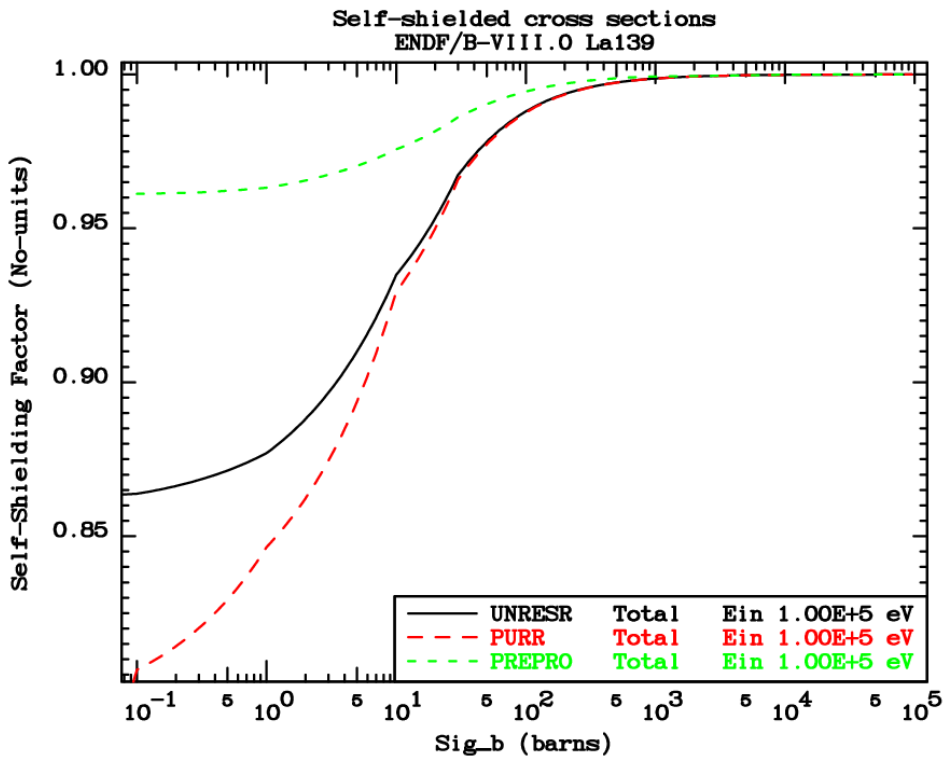

Figure 6: Self-shielded cross sections as a function of the Bondarenko dilution cross section for incident neutrons of 100 keV, produced by different methods.

5 CONCLUSIONS

The analysis of the model problem and the self-shielding treatment on ^{139}La from the ENDF/B-VIII.0 library leads to the following conclusions

- Cross sections of ^{139}La at the RRR/URR boundary have a large discontinuity.
- The effect of self-shielding in deep penetration problems for ^{139}La is important.
- Different methods of using the URR parameters lead to significantly different results.
- The method of generating multi-band parameters in PREPRO is based on extrapolation from the RRR and gives results that look physically reasonable. Other methods tested in this work produce leakage spectra with unphysical behavior.

The model problem can be used for testing other evaluations in general purpose libraries. Hopefully, the problems identified in this work related to the content of evaluated data files, as well as the methods for the treatment of self-shielding will stimulate additional work to remove inconsistencies and unphysical behavior, inspiring greater confidence in the calculated results in general.

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