An assessment of neutron resonance data for mid-mass isotopes

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Abstract. A survey has been conducted of the resonance data available in the major evaluated libraries for a range of mid-mass isotopes. Although many isotopes have data derived from experimental measurements and rigorous analyses, the data for some others, particularly for isotopes that are unstable, are purely theoretically generated, e.g. via the use of the TARES code.

A subsequent project has developed a suite of automated tools to rapidly inspect the resonance data available for a specified isotope. These tools calculate a range of values and distributions for the available data (e.g. cumulative number of resonances versus neutron energy) and use a comparison against expected theoretical values (e.g. a Porter-Thomas distribution) to suggest their physical validity or otherwise.

The motivation for this study, the tools developed, and results for a number of isotopes, are presented in this paper.

1 Introduction

A number of new nuclear data evaluations are being performed at AWE. These evaluations, for a range of mid-mass isotopes, will include data for several unstable isotopes. The nuclear data required at higher energies are generated by fitting TALYS calculations to available experimental data [1]. Although the main focus is on higher energy threshold reactions, data for lower energy reactions must still be present in the evaluation.

Cross sections for low energy reactions are typically dominated by resonance behaviour. An example cross section with a resolved resonance region (RRR) present is shown in Figure 1. The data for these resonance regions are stored as sets of resonance parameters from which the cross section may be reconstructed. Evaluations for resonance regions require a different approach to those performed at higher energies where the cross section varies smoothly and mean-field potential models, e.g. the Optical Model, can be used in calculations.

For these new mid-mass evaluations, if rigorously evaluated resonance parameters are already present in an existing evaluation, these are adopted. A survey has been conducted of the resonance data available in the major evaluated libraries for approximately 40 mid-mass ($A \approx 90$) isotopes. Unfortunately, for many of these isotopes resonance parameters do not exist (as no evaluation exists) or else they are not based on a rigorous evaluation methodology.

The work documented in this paper seeks to answer the question: “If good resonance data are not available in an existing evaluated library, e.g. ENDF/B, JEFF or JENDL, what is the best way to easily generate physically realistic data?”

2 Resolved Resonance Regions

Ideally, the evaluation of the resonance region of an isotope would involve a combination of experimental data and detailed theory. Typically, this would involve an R-matrix fit of transmission and time-of-flight measurements in order to extract parameters for the resonance region. Unfortunately, measurements of this sort are generally not available for unstable isotopes and so other approaches must be used.
2.1 Alternative sources of resonance parameters

Figure 2 shows examples of RRRs created using a range of alternatives to the full R-matrix fitting approach. Brief descriptions of these different methods are given below.

**Smooth** With no knowledge of the true RRR available, a smooth cross section is used instead. This cross section is derived from a (possibly calculated) thermal capture cross section. This method has the advantage that no physics is “made up”, but its results are obviously incorrect and also fail to satisfy a number of statistical metrics which physically correct RRRs should obey (see Section 2.2).

**Single Resonance Approximation (SRA)** A single wide resonance is created which approximates the average behaviour of a physically correct RRR [2]. The SRA is obviously not correct (for all but very light nuclei), but if the resonance is carefully created, it can actually satisfy a range of RRR metrics (see Section 2.2).

**Surrogate** A full set of resonance parameters is simply “transplanted” from a neighbouring isotope. The donor isotope should be physically similar with a set of rigorously evaluated resonance parameters.

**Radiator** This method is one available within the 	extsc{tares} code [3]. 	extsc{tares} is used to create resonance parameters (and also uncertainties) to complement smoothly varying higher energy cross sections calculated via the 	extsc{taly} nuclear reaction code. A set of uniformly spaced resonances is created with the neutron strength function calculated using the “extreme” compound nucleus model.

**High Fidelity Resonance (HFR)** Available within the 	extsc{tares} code, this method uses average unresolved resonance region (URR) parameters, which can be calculated using 	extsc{taly}, as inputs. 	extsc{tares} passes these URR parameters to the 	extsc{calendf} code [4] (present within 	extsc{tares}) which uses a “random ladder” method to produce RRR parameters. 	extsc{tares} then adjusts the RRRs to reproduce a desired thermal capture cross section.

2.2 Metrics

In the absence of experimental data (either differential or integral), the question arises of what a physically valid RRR should look like. A number of different authors have proposed metrics (in the form of distributions of various quantities) which may be used to assess the suitability of RRRs. In particular, each can be useful for indicating that a dataset has missing resonances and a number can also identify the energy region(s) where these missing resonances may be. The different metrics are described briefly below.

**Porter-Thomas distribution** This distribution, introduced by Porter and Thomas in 1956 [5] based on an extension to the work of Harvey et al. [6], gives the expected frequency distribution of resonances as a function of neutron width (divided by the average width). Figure 3 shows a theoretical Porter-Thomas distribution compared against the calculated distribution for the $^{89}$Y evaluation found in the JEFF3.3 library [7].

**Wigner distribution** This distribution was proposed by Wigner in 1957 [8] and can be used to describe the distribution of compound nucleus state spacings and therefore the spacings of resonances.
Cumulative number of resonances against energy
This simple distribution can be estimated from a knowledge of the average resonance spacing and neutron strength function [9].

Cumulative neutron widths against energy This distribution is similar to the previous, except the cumulative neutron widths multiplied by a spin factor are plotted as a function of energy.

Ratio of s-wave to p-wave resonances The two distributions above are limited to s-wave resonances. Neutron strength functions can also be calculated for other possible resonance spins. The cumulative ratio of s- to p-wave (or even s- to d-wave, etc) resonances can be plotted as a function of energy and compared against the resonance parameters in an evaluated dataset.

The RRs produced in this study have been compared against several of these metrics as part of the assessment process.

3 Benchmarking
Whether or not a generated RRR satisfies the various metrics described above is one way of assessing the performance of a method for creating RRRs, but a more thorough assessment can be made using a suitable integral benchmark.

A series of 1950s experiments, led by C.C. Byers, involving the irradiation of different target foils within critical assemblies were chosen as the benchmark model for this study [10, 11]. In these experiments, performed at the Godiva, Jezebel and “Water Boiler” assemblies, a foil of atomic mass $A$ was inserted into the critical assembly and following the irradiation period, the number of $A+1$ isotopes created via neutron capture reactions was measured from the rate of $\gamma$-decay. This experimental setup was chosen as a benchmark due to its sensitivity to the neutron fluence at resonance energies and its measured output being directly proportional to the neutron capture cross section (which is dominated by resonance behaviour at low energies).

The Godiva experiments were modelled using the fispact-II inventory code [12]. Using each of the methods listed in Section 2.1, resonance parameters were generated for each isotope investigated in this work. These resonance parameters were combined with high energy cross sections calculated using TALYS and processed into a single nuclear data file.

The 11 isotopes studied in this work span a range of masses from $A=85$ to $A=103$.

Table 1. Results of calculations of the Byers benchmark for $^{89}$Y

<table>
<thead>
<tr>
<th>Method</th>
<th>$N(90^{g}Y)$</th>
<th>$N(90^{m}Y)$</th>
<th>$\delta(L)%$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ENDF/B-VIII.0</td>
<td>2.726x10^{9}</td>
<td>7.194x10^{7}</td>
<td>n/a</td>
</tr>
<tr>
<td>Smooth</td>
<td>2.678x10^{9}</td>
<td>7.179x10^{7}</td>
<td>-1.710</td>
</tr>
<tr>
<td>SRA</td>
<td>2.688x10^{9}</td>
<td>7.187x10^{7}</td>
<td>-1.338</td>
</tr>
<tr>
<td>Radiator</td>
<td>2.623x10^{9}</td>
<td>7.130x10^{7}</td>
<td>-3.714</td>
</tr>
<tr>
<td>HFR</td>
<td>2.695x10^{9}</td>
<td>7.192x10^{7}</td>
<td>-1.084</td>
</tr>
<tr>
<td>Surrogate</td>
<td>2.858x10^{9}</td>
<td>9.412x10^{7}</td>
<td>5.530</td>
</tr>
</tbody>
</table>

Unfortunately, measured results only exist for a small number of isotopes of interest to this study. In addition, a number of experimental details were unavailable. Therefore, rather than match the fispact results to experiment, they have instead been compared against results calculated when using a RRR from an evaluated library. This evaluated library, ENDF/B-VIII.0 [13], is therefore assumed to be “correct” and the other methods are compared relative to it.

Table 1 shows the benchmark results calculated for each method for $^{89}$Y. $N(90^{g}Y)$ and $N(90^{m}Y)$ are the number of atoms created of the ground and metastable states respectively of $^{90}$Y. $\delta(L)$ gives the percentage difference between the sum of these atoms and the result calculated using the ENDF/B-VIII.0 reference library. The $\delta(L)$ results are also illustrated in Figure 4.

The results for all of the isotopes studied are shown in Figure 5. The results for each method are displayed as
normal distributions generated from the calculated average $\delta(L)$ and standard deviation.

As may be seen in Figure 5, the HFR method was found to produce results that were closest to those of the reference library. The HFR method also performed well when compared to the various metrics described in Section 2.2. The radiator method was found to be the worst performing. The performance of the surrogate method is highly dependent upon the choice of donor isotope. It may be that its results would improve if different choices were made.

4 Conclusions

A number of different methods for inexpensively creating resonance parameters for isotopes lacking rigorously evaluated parameters have been investigated. The parameters generated using these methods have been tested against a number of metrics and also used in calculations of a critical assembly neutron capture benchmark.

The High Fidelity Resonance method, available within the TARES code, was found to be the best performing method, with the “Radiator” method the worst performing. However, it should be noted that only a single benchmark model was studied along with only a relatively small subset of mid-mass isotopes.

A future study using a greater range of benchmarks and isotopes would be beneficial in order to confirm, or otherwise, the results of this study.

Acknowledgements

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References