Report: LLNL-TR-2008244

Correct Interpretation of ENDF-102 Definitions for Resonance Effects

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Prologue

My Uncle Willie circa 1600 wrote “What’s in a name; a rose by any other name would smell as sweet.” I fear in this case we have a somewhat similar problem in that we may be using the same word but are not using the same definition; specifically, the word **Unresolved**. The simplest physics definition as it applies to neutron resonances, is the energy point where we can no longer see/measure ALL – let me repeat that – ALL - of the individual resonances. That seems simple and clear, but the question is: how to represent resonances beyond this point in order to accurately reproduce the effects we have seen in measurements and expect/need to reproduce in our applications. We know there are more, unseen resonances, otherwise we wouldn’t say Unresolved.

The ENDF approach is well defined in ENDF-102 and simple: for ENDF data the only way to represent Unresolved data is by using a theoretical model to define the distribution of resonances, including those that are too narrow to measure (i.e., are unresolved). It is important to note that in ENDF this is the one and only Unresolved model, e.g., **there is no provision in ENDF to accurately define individually ALL resonances above the Resolved energy range – by ALL here I mean both those that we can measure and those that we cannot individually measure, but that theory and integral measurements tells us are present.**

An alternative approach, which would appear to be equally valid, would be to include the latest measured data as tabulated energy expendent data extending upwards in energy above the Resolved energy range. In this approach the evaluation would not include an ENDF style Unresolved energy range; it would only include a Resolved resonance region, followed by tabulated higher energy points, representing the resonances that could be measured beyond the Resolved range. But an important point to note: By listing these resonances above the resolved energy **one admits that at least some resonances in this energy range are missing as Unresolved**; i.e., they are too narrow or overlapping to measure.

The purpose of this paper is to illustrate that the later approach, while done with good intentions, and appearing to be valid/adequate in plots, **does not meet the need of our engineering applications**. Why? As we will see below, of these two possible approaches, only the ENDF use of a model to statistically include the missing, i.e., unresolved, resonances, can meet our engineering needs to reproduce the integral effects we have measured and understand. Only with this statistical model can we predict and include in our calculated results the important effects of temperature (Doppler broadening), and energy integrals (self-shielding).

Below I will first present results using two ENDF/B-VIII.1 evaluations, U235 and U238, that use the correct ENDF-102 definition of an Unresolved resonance region, using a statistical model to include the effects of resonances that theory predicts are present, but are too narrow to measure. These two evaluations reproduce the expected temperature (Doppler) and energy integral (self-shielding) effects that we expect. Next I will present results using one ENDF/B-VIII.1 evaluation, 26-Fe-56, that does not use an ENDF-102 Unresolved resonance region; instead above its Resolved energy range it lists many tabulated energy points, that look like measured data, but by definition, since they are included above the ENDF Resolved energy range there are missing Unresolved resonances, i.e., there are missing the resonances that are too narrow to resolve, i.e., are unresolved. **My conclusion, and I hope yours, is that the below figures illustrate that this approach does not reproduce the temperature and energy integrals that we expect and need to accurately calculate results for our fission reactor calculations. As such this approach should not be used in ENDF formatted evaluations.**

History 101

When Henry Honeck invented the ENDF format, circa 1965, he based it on his personal knowledge and experience from both producing and using evaluated nuclear data. ENDF was to a large degree based on the earlier UKNDL format. Both formats/systems were designed to allow nuclear data for nuclear fission applications to be represented in a simple computer independent, character based 80 column computer card format, that was easy to exchange between computers/labs.

The important characteristics of ENDF that I will focus on here are the representations of **nuclear resonances.** The reason I have tried to clarify the correct ENDF definitions is because **it is these definitions, and only these definitions, our processing/application codes assume the data are using, so we must all obey these definitions to accurately perform fission reactor calculations.**

I fear that recent evaluations are drifting away from the original purpose of ENDF, and in particular they are not representing nuclear resonances – and related data – in a form that can be correctly interpreted by us and our codes and accurately used in today's applications. **I can only hope that it is not too late to correct this problem and get us back on the path to improving ENDF by ALL of us agreeing to use exactly the same ENDF-102 defined rules and definition.**

Honeck's definitions of Resolved and Unresolved are based on **Engineers definitions** and needs. Unfortunately, based on my recent survey of ENDF formatted cross sections it would appear that many evaluations are using **Nuclear Physics definitions**. How do they differ? In Henry's **Engineering definition** individual resonances are only allowed to be defined in the Resolved resonance range. Above the resolved range Henry defined an Unresolved resonance range, where by definition we cannot uniquely define each and every individual resonance; hence the definition Unresolved: here we can only use a statistical model. The alternative **Nuclear Physics definitions** approach is to simply list in the ENDF format what we can measure. **Based on the results I show below, sorry to say this Physics approach does not reproduce the important integral results we expect, so we cannot use it in our applications and still expect to produce accurate results.**

The below examples of U235 and U238 illustrate the correct use of this **engineering model** that we need to produce accurate results in our applications. Unfortunately, today it appears that some evaluators use a different model above the resolved resonance region. What I find in many evaluations is simple tabulations of resonance that were measured above their defined Resolved range. **This seems like a perfectly reasonable definition of Unresolved, but unfortunately it is not the ENDF definition that we require.** I will show below using 26-Fe-56 as an example, a plot of the data may appear reasonable, but a calculation of the effects of Doppler broadening and self-shielding demonstrate that the narrow unmeasurable (i.e., unresolved) resonances are by definition not include in any measured Unresolved data range, so this simple tabulated data will not produce results to the accuracy we require in our applications, e.g. calculations of a Doppler and self-shielding effects that both theory and integral measurements tells us really exists, that we must reproduce in order to accurately calculate the safety of any fission based system.

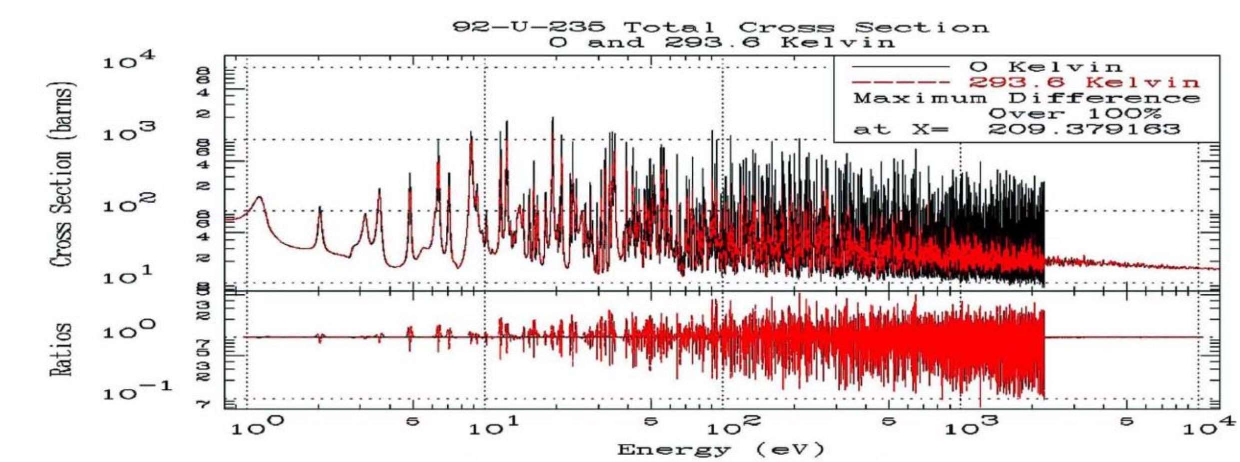
By definition, self-shielding is a multi-group effect, based on energy averages. Here I have used the TART 616 group structure, which uses a uniform log spaced 50 energy groups per energy decade between 10^{-5} eV and 20 MeV; there is no preference to any specific energy range. Note, in our applications we are only interested in average/integral results, not results at any one energy. Hence, these energy average are representative of what we need to calculate in our applications.

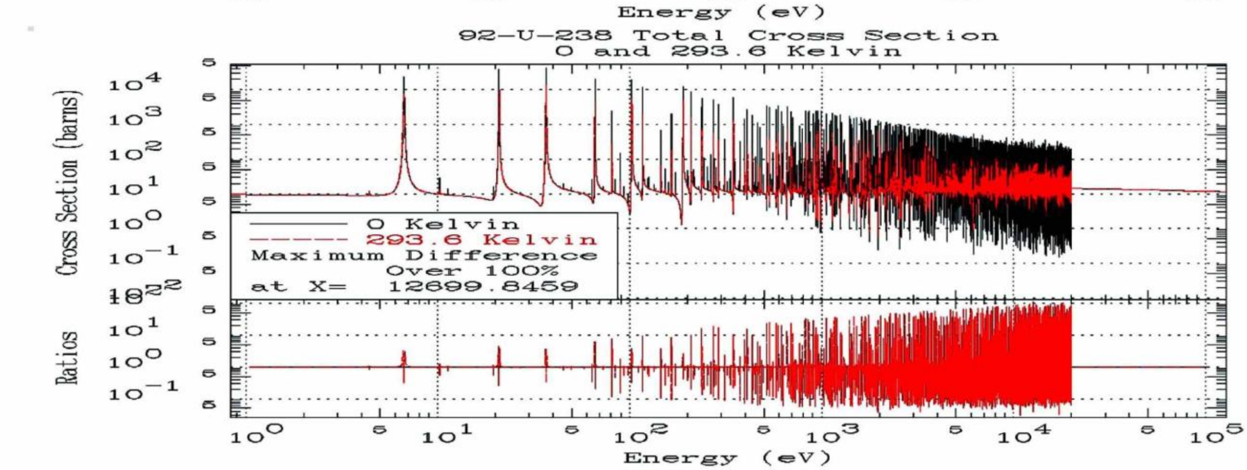
Effect of Doppler Broadening

To give you, the reader, a feeling for how important Doppler broadening effects neutron cross sections, below I show results for ENDF/B-VIII.1 U235 and U238 Total cross section comparing the data at 0 Kelvin and 293.6 Kelvin (20 Celsius = room temperature). The important points to note based on the ratios (ratios are shown in the bottom part of plots):

1) In the **Resolved** resonance region, the broadened cross section can be **up to 100 times HIGHER** near the minimum between resonance, and **up to 20 times LOWER** near resonance peaks. U235 has **743,503** tabulated energy points at 0 K, and **110,829** at 293.6 K. U238 has **1,787,916** tabulated energy points at 0 K, and **273,142** at 293.6K. Obviously there are enormous differences in the cross sections even between 0 and 296.3 Kelvin.

2) In the **Unresolved** resonance region, the **Unshielded Energy Average** cross section, shown in these plots, is smoothly varying, using the correct ENDF-102 definition, that the unresolved region defines only the average distribution of resonances; this distribution statistically includes the very important narrow resonances, too narrow to measure individually; hence the name **Unresolved**. **Based on ENDF-102 definitions there are NO individually measured resonances in a properly defined ENDF-102 Unresolved region; only statistical distributions that includes unmeasurable narrow resonances.** By a convention that I adopted in 1970, plots of ENDF unresolved data are Unshielded, energy average data, which usually appear to be very smooth.





Effect of Self-Shielding

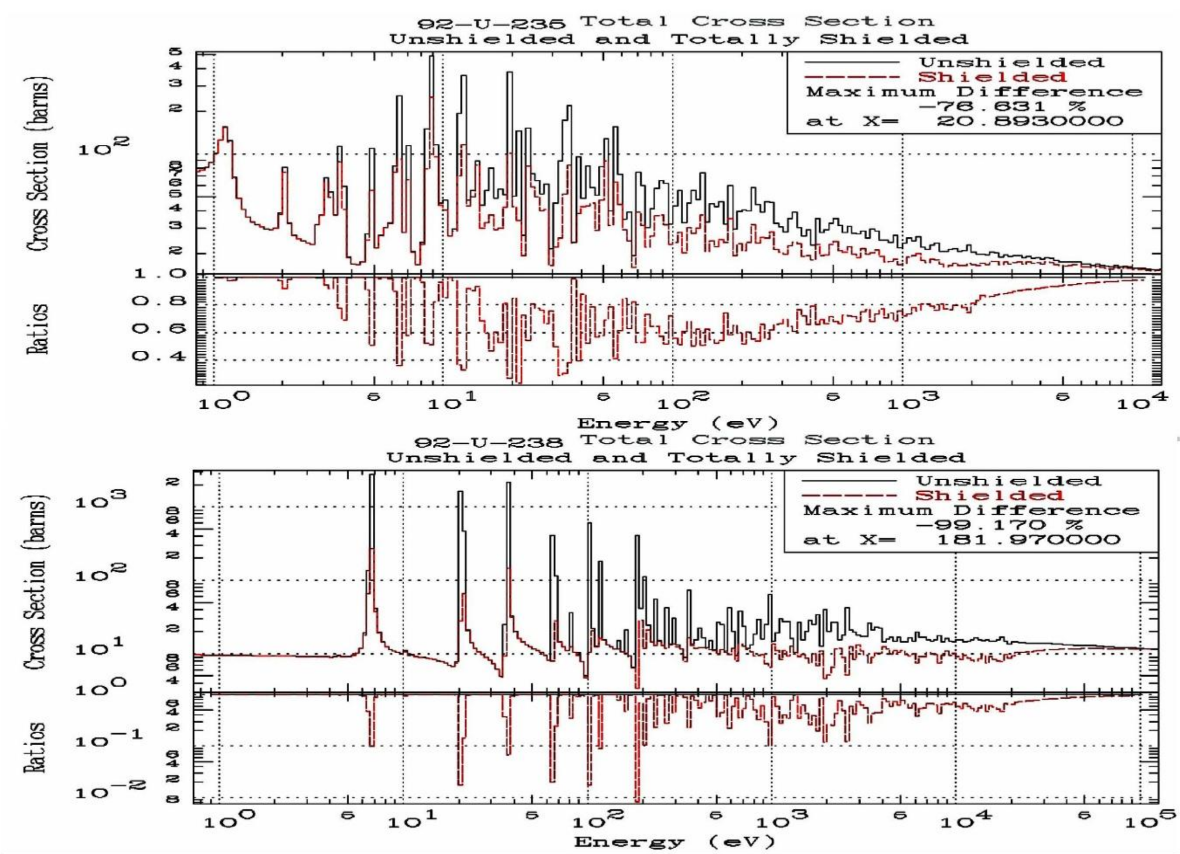
To give you, the reader, a feeling for how important Self-Shielding effects neutron cross sections, below I show results for ENDF/B-VIII.1 U235 and U238 Total cross section comparing **Unshielded** and **Totally Shielded** data at 0 Kelvin. The important points to note based on the ratios (ratios are shown in the bottom part of plots):

1) In the **Resolved** resonance region, the U235 Shielded cross section can be as little as only 24% of the Unshuelded cross section (a factor of 4 difference). In the Resolved the U238 Shielded cross section can be less than 1.0% of the Unshielded (a factor of 100 difference), over a narrow energy range.

2) In the **Unresolved** resonance region, the Shielded can be as little as 80% of the Unshielded cross section – I repeat, this is based on nuclear resonance theory to include narrow, unmeasurable resonances.

3) As expected based on the unresolved resonance model being used, shielding in the unresolved region is much more uniform in energy than shielding in the Resolved range, which is caused by individual resolved resonances.

4) From this log Energy plot, it is not obvious, but the Unresolved region is almost 10 times longer in energy than the Resolved. Basically, the last decade of energy in these plots is the Unresolved energy range (90% of the entire energy range of these plots), making it more important than you might think from these plots.



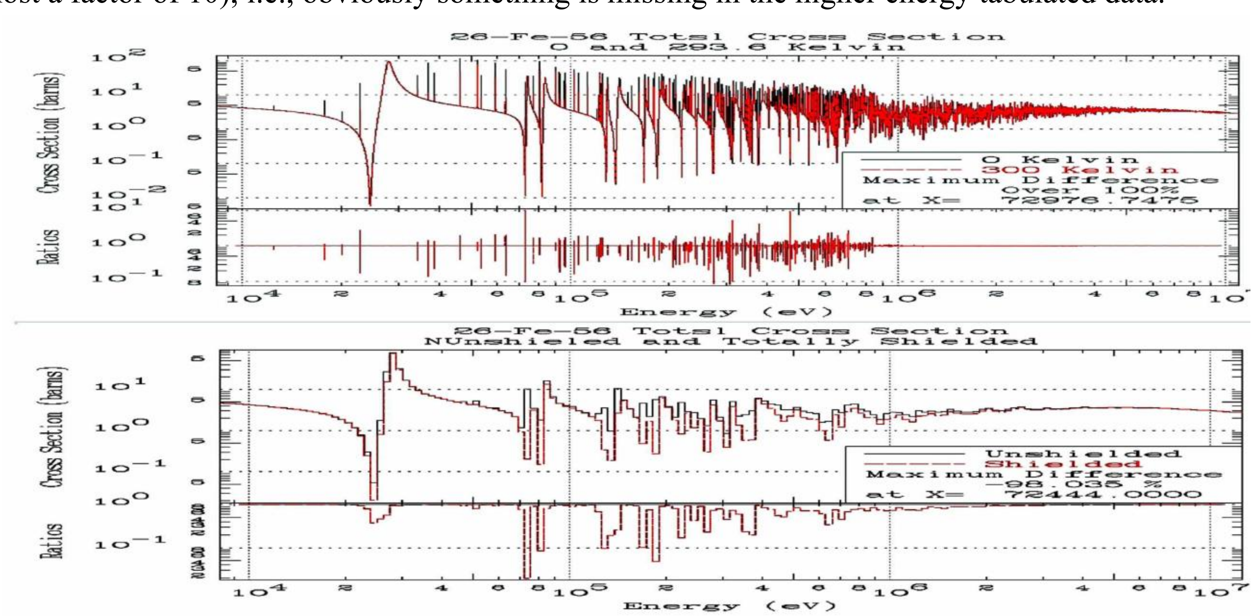
Comparison to an Evaluation that Do NOT follow ENDF-102 Rules

The above U235 and U238 results are examples of two evaluations that follow/obey ENDF-102 definitions and conventions, specifically ENDF-102 definitions of Resolved and Unresolved resonance regions. Below is an example that does not follow these conventions. The example I use here is ENDF/B-VIII.1 26-Fe-56 that includes only a **Resolved** energy range; there is **no Unresolved** range. However, there are many tabulated resonance like energy points above the Resolved range, and these appear to be very detailed until we look at Doppler broadening and self-shielding.

Compared to the above U235 and U238 results, based on the below plots showing 26-Fe-56 Doppler broadening and Self-Shielding.

1) We can clearly see Doppler broadening in the **Resolved** resonance region, up to 800 keV. Above this energy range (the so called ENDF high energy tabulated data), there is virtually no effect of Doppler broadening for what appears to be detailed energy tabulated resonances. This plots tells us that the narrow resonances predicted by resonance theory are not included in this evaluation, i.e., these very narrow resonances, that are missing from measurements, have the greatest effect on Doppler broadening and Self-Shielding.

2) These tabulated higher energy data may be based on actual measured results, but hopefully these figures showing the resulting effects on Doppler broadening and Self-Shielding demonstrate why evaluators cannot simply copy experimental results to the ENDF format and call it "evaluation"; they must perform actual "evaluation" to add the missing very narrow unmeasured resonances, to allow this data to be accurately used in applications. Alternatively, evaluators can convert the mass of tabulated higher energy data into a few points of ENDF Unresolved data. Also note the decrease in the height/depth of fluctuations above the end of the Resolved at 800 keV (a discontinuity of almost a factor of 10); i.e., obviously something is missing in the higher energy tabulated data.



Epilogue

First, we should all be aware that what neutrons see and interact with are the cross sections shown here: Doppler broadened and self-shielded in the Laboratory frame of reference; not the “cold” (0 kelvin) data in the center-of-mass system included in ENDF evaluations as distributed, i.e., ENDF raw data needs processing before it can be used by our application codes. I have not included any references in this report because I did not want to distract, you the reader, from the one and only purpose of this brief report: **The nuclear data needs of fission reactors cannot be met solely based on measured continuous energy dependent data; energy integral (e.g., multi-group) data is required to accurately reproduce important temperature and self-shielding results.**

At first this may seem at odds with intuition, where measured results are considered to be the most accurate and reliable data to use in our evaluations. But in fact, it is not at all a contradiction since **INTEGRAL energy results have been measured that reproduced the self-shielding effects I described above**; these are results that are not present in the 26-Fer-56 evaluation because the narrow, unmeasured resonances that theory tells us exist are not included. I will mention the measurements of Bramblett-Czirr, who measured the transmission of neutrons through various thickness of several materials. Without any self-shielding effects we would expect a simple exponential attenuation versus thickness, i.e., a straight line on a semi-log plots of thickness vs. transmission. However, due to actual self-shielding this is not at all what they saw in their measurements, i.e., they clearly measured self-shielding = **it is real and has been measured**,

I asked Bart Czirr how they selected the energy ranges that they used in their measurements, but he did not know/remember. But I recognized the group structure that they used as the Russian ABBN fast neutron groups, of three (3) groups per energy decade. The ABBN data is from well over 50 years ago, and they managed to reproduce self-shielding in applications using Nikolaev’s sub-group method; Nikolaev is the N in ABBN. I recognize the connection after I listened to a presentation by Leo Levitt describing his Probability Table Method (PTM), to reproduce self-shielding in properly defined ENDF unresolved region. I immediately saw that Leo’s PTM could be extended to all energy ranges; what I called my mufti-band method. Only after I published a report on multi-bands, was I contacted by Nikolaev pointing out that what I proposed was in fact identical to his sub-group method; Nikolaev is indeed the earliest one I could trace who recognized and presented a method to solve the problem of accurately reproducing self-shielding in applications – **yes, he both measured and calculated real self-shielding.**

My point here is that the **energy integral self-shielding and how to accurately model it for use in applications was well understood over 50 years ago.** That is why Henry Honeck’s defined ENDF Unresolved resonance region model was so important then and today. Other nuclear data formats, such as ENDL, that use only tabulated energy dependent data (it has no models) cannot reproduce energy integral Doppler and self-shielding effects described here. ENDL was used very successfully for many years by Los Alamos and Livermore with their Monte Carlo codes MCNP

(LANL) and TART (LLNL), for fast neutron applications, where there is little or no resonance structure, and thus little or no self-shielding. When these codes were applied to lower energies (where they were not originally designed to be used) they often continued to produce the same answers, **but what they both produced was the same wrong answer**; because they did not correctly model missing narrow resonances. Only after MCNP and TART added models did they both reproduce reliable lower energy results. MCNP added Leo Levitt's PTM and TART added my multi-band method. Today MCNP and TART calculated results agree closely. I hope that this a not too subtle WARNING about "garbage-in = garbage-out" – **regardless of how good your application code is your results can be no better than the quality of the data that you use**.

My punchline is that we have known about and accounted for energy integral effects for well over 50 years, but I fear that today's evaluators are no longer aware of the importance of what ENDF defines as Unresolved (i.e., a nuclear model), and they think/assume that by including more and more resonance structure measured to higher and higher energies they are improving ENDF evaluated data for use in our applications. In fact, they are merely making calculations run much longer without reproducing the Doppler broadening and self-shielding effects that nuclear physics predicts and based on integral measurements we know are truly present.

For example, ENDF/B-VIII.1 26-Fe-56 total cross section without the MF=2 resonance contribution includes 15,151 tabulated energy points up to high energy. Yet the above plots prove this does not produce the expected Doppler and self-shielding effects. In contrast **if evaluators followed Honeck's Unresolved model they could replace these 15,151 points by a few hands full of ENDF unresolved parameters, that would reproduce correct Doppler and self-shielding effect that we physically expect and need to model our applications.** I will merely mention that the most widely used unresolved model in earlier version of ENDF/B is the so called "the picket fence" model, where unresolved average widths and spacing become constant at higher energy, which is so easy to define using the correct Honeck ENDF definition of unresolved,

Many people claim that history is cyclic. I can only hope that this is not true of ENDF/B. We have come so far through eight (VIII) major releases and in my humble opinion by versions V or VI we had converged, in the sense of meeting most of our fission reactor needs, to the point that many users lost interest in updates. But theoretical and experimental physicists did not lose interest and continued to update the data in what they assumed would better met the needs of our applications. But I fear that what these recent changes have actually done is move ENDF away from Honeck's ENDF models, back toward ENDL, that uses no models; today evaluators who only use more and more energy dependent measurements, I fear are directing us back to where we were 50 years ago.

Let me suggest we work together to avoid this happening by understanding and conforming to Honeck's original ENDF definitions and models - they have worked for over 50 years; please do not change the rules that we and our computer codes now understand.

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