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Unfolding Cross Sections: A Brief Introduction

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Overview

Unfolding Cross Sections has been around forever, so there is nothing new in this report. I only authored this report because I fear that the current generation of ENDF data creators and users may not be familiar with this concept. This will be a brief introduction to unfolding, so I will only present one example, namely, ENDF/B-VIII U235. Let me stress that in selecting this example it was only because of the obvious importance of U235. In this selection I am not making any judgement as to the quality of this evaluation. Indeed, as I will keep reminding readers throughout this report, in my opinion the evaluators did an excellent job, and this evaluation meets the needs of many users. But it does violate ENDF-102 [1] that states MT=5 can be used for complex reactions at high energy. This evaluation uses MT=5 all the way down to the traditional ENDF lower energy limit at 1.0e-5 eV. There are no complex reactions at 1.0e-5 eV and this is certainly not high energy. To illustrate unfolding I will start from what I call their current U235 BEST physics evaluation and present what I call my BEST engineering evaluation, that better meets my needs - and more importantly the needs of the codes I use to process and use ENDF data. You, the reader, are free to select either - or neither - for your personal use. ENDF has been such a GREAT success because of the close bond between data producers and data users, who have supplied user feedback to improve the next generation of ENDF data. Here I am merely one of those users, and this is my feedback.

What is ENDF?

Let me start by defining what ENDF/B is and is not. To me ENDF-102 [1], the ENDF Bible, is an **Engineering User's Manual**; it is not a physics text book. Obviously, the evaluations in ENDF are based on a combination of measurements, theory, and when all else fails, the evaluator's best "guesses". ENDF is designed as an interface between physicists. who prepare the evaluations, and

engineers, who use the data in their applications. This is an important point to understand that in order to allow evaluations to be used in applications they must be complete. ENDF is NOT intended as a storage place for physics ideas. The important difference between the **BEST physics** and **BEST engineering** ENDF evaluation is that in physics we have the luxury of admitting "I do not know", whereas in ENDF to be useful in applications we do not have this luxury. For anything that the evaluator does not know an extremely important part of each ENDF evaluation, is that the evaluator **MUST use their knowledge to provide their BEST "guess"** to make their evaluations complete and uniquely useful in **engineering applications**.

What has made ENDF such an International success is that everything is UNIQUELY defined in ENDF-102. No claim is made that the equations and conventions defined in ENDF-102 are the BEST physics. For the use that ENDF is intended, in **engineering applications**, ENDF-102 need not be the BEST physics. It need only be unique and easy to understand by both physicists who prepare the evaluations and engineers who use the data, **AND most important everybody involved MUST agree to strictly follow the rules defined in ENDF-102.** One of the biggest problems we have had throughout the history of ENDF is when data producers or users think they know better than the rules defined in ENDF-102. **Usually they are right; they may know physics better.** But they can cause havoc if they try to use their knowledge if it violates ENDF-102 rules. To work EVERYBODY must obey the ENDF-102 rules, e.g., an evaluator cannot use their own "better physics" definition of resonance parameters, because our stupid computer codes will not understand and will use the ENDF-102 definitions, which can lead to obvious rubbish results, or worse, results that are not so obviously rubbish and we believe them.

Until recently this was not a problem for ENDF. The ENDF-102 Bible uniquely defined everything, and millions of dollars were invested to exactly follow these rules to produce reliable application results. The heart and soul of ENDF was MF=3, cross sections. The cross section for each and every individual reaction was defined in MF=3. For each MT (reaction) defined in MF=3, secondary particle information was defined in MF=4 (angular), MF=5 (energy), MF=6 (coupled energy-angle). This made it simple for our millions of dollars' worth of ENDF processing and application codes to uniquely understand, follow and accurately use the data in our applications.

Then MT=5 (n, anything) was introduced; what I call "I don't know". In principle this should not be a problem for the applications that ENDF was designed to handle, namely fission, and later fusion systems, since ENDF-102 states that MT=5 may be used for **COMPLEX REACTIONS AT HIGH ENERGY**. I assumed, and most experienced evaluators, interpreted this to mean ideally above 20 MeV, where there are no fission or fusion neutrons – at least not enough that engineers need be concerned about. The problem is that some evaluators used MT=5 "I don't know", all the way down to the traditional lower energy limit of ENDF at 1.0e-5 eV. To me this was first of all an obvious violation of ENDF-102, but more importantly it had the potential to totally confuses our million dollar codes that use ENDF data. When I use a Monte Carlo code to

track neutrons collision by collision, in the past at each collision ENDF data in MF=3 uniquely defined the outcome of each collision, so I could continue tracking and accumulating results. I am sorry but my codes are too stupid to understand what it means when the outcome of collision is "I don't know". Whatever I decide to do in this case, may not be what you decide to do in your code, hence our results are no longer unique. This is a problem that must be fixed at the source, in the evaluation, so that we again guarantee unique ENDF results. Fortunately, for all of the cases that I have looked at in ENDF/B-VIII the solution is relatively simple to uniquely define the needed MF=3 cross sections using Cross Section Unfolding. This can be done using nothing more than the current data included in the evaluations; no additional nuclear model codes, or anything else is needed. As we will see below the evaluators of ENDF/B-VIII U25 did an excellent job of defining everything in what a call their BEST physics evaluation; that is everything I need for my personal use in what I call my BEST engineering evaluation.

Before I start let me stress again that for the current ENDF/B-VIII data in my opinion the evaluators who produced this low energy MT=5 data did a great job. It is only through their efforts to include in their evaluations details in MF=6 defining secondary light particles and isotopes produced by MF=3/MT=5 "reactions", that have been able to unfold cross sections. In my opinion the difference between what they produced and what I propose are a perfect example for the difference between evaluations that are based on the **BEST physics**, what we have today, and the **BEST engineering** solution, which is what I propose in order to make these evaluations acceptable for use by my codes in **engineering applications**. Again, in BEST physics we can say "I don't know" (MT=5), whereas in BEST engineering we do not have that luxury and must uniquely define everything for use by our stupid million dollar codes.

My Background

Why am I writing this? Why should you, the reader, care about my opinion; **be assured this is strictly my opinion**. It is because of my background in ENDF throughout its entire history. By the time I completed my doctoral thesis on integral neutron transport [5] in 1967 I realized that the biggest barrier to obtaining accurate answers to neutron transport problems was the lack of accurate neutron interaction data; regardless of how accurate our transport codes were, without accurate nuclear data we were in a "garbage in = garbage out" situation. In an attempt to contribute to solving this problem the first job I accepted was at what later became the National Nuclear Data Center (NNDC), Brookhaven National Laboratory. At the time the Evaluated Nuclear Data File (ENDF) was in its infancy; the first version of ENDF/B had just been released. To my knowledge this was the first attempt to establish a U.S. National neutron data library for use in fission and later fusion applications. By 1970 I understood ENDF so well that I used it as a model to design the current X4 (EXFOR) format, for experimental data, so that we could have access to as much experimental data as possible for use in our ENDF evaluation efforts. To me the big difference between ENDF and EXFOR is that ENDF uses fixed units (energy eV, cross section, barns), whereas I designed EXFOR to allow any units (easily accommodating whatever units the measured

data is published in). After working at NNDC, BNL for five years I moved to Lawrence Livermore National Laboratory (LLNL) and returned to work on my first love: neutron/particle transport using the TART [2] Mone Carlo transport code.

Since 1967 I have worked on all eight versions of ENDF/B, starting with the already released version of ENDF/B (no roman numerals after the name), up until today's ENDF/B-VIII. I have contributed computer codes PREPRO [3] to perform standard operations to prepare ENDF formatted data for use by cross section processing codes and in turn application codes. On what I think of as the other side of the fence, I have prepared evaluated data and updated/corrected evaluated data. Today I provide the sole support for the ENF/B-VIII atomic electron and photon interaction cross sections, EPICS2023 [4]. In summary, by today for over 50 years I have been working on ENDF related codes and data.

I have been retired for 15 years, but I have continued my work without any monetary compensation in order to keep my mind active. Today I support: 1) EPICS2023 [4] atomic electron and photon data, 2) PREPRO2023 [3] ENDF Pre-processing codes, and 3) TART2022 [2] Monte Carlo coupled neutron-photon transport code. Only recently did I add PLOTTAB graphic output to my PREPRO/SIXPAK code; for the first time I am now able to see MF=6/MT=5 data, as shown in this report. After seeing this data for the first time I can really appreciate what a tough job the evaluators had, and what a good job they did, since their MF=6/MT=5 data includes everything that I need to unfold the U235 MT=55 cross sections. I have always said "One picture is worth a thousand words". In this case the pictures of this data prompted me to produce well over a thousand words in this report. That is my pedigree, and I think it is fair to say I have as much, if not more, experience with ENDF than anyone.

Unfolding Cross Sections

Here I will attempt to use my experience to help explain why I personally feel that the recently introduced MT=5 (n, anything) should be restricted to exactly what it says in ENDF-102 [1], the ENDF Bible: **COMPLEX REACTION AT HIGH ENERGY**. I will use cross section unfolding to illustrate how simple it is to accomplish this using one example of current ENDF/B-VIII U235 evaluation where, in my opinion, MT=5, is being misused, extending it down to the traditional lower limit of ENDF at 1.0e-5 eV. This is but one example but be assured that after examining ENDF/B-VIII in detail I can state that **there are no evaluations in ENDF/B-VIII that requires MT=5 to be misused for lower energy; I repeat, there are no complex reactions at low energy.**

First let me briefly explain the objective of cross section unfolding as I will use it in this report. Starting from an existing ENDF/B-VIII evaluation where the evaluators extend MT=5 down to 1.0e-5 eV, I will demonstrate how using nothing but what is currently included in the evaluation, I will start from the existing MT=5 data moving from low energy too high to define one reaction at a time, leaving the remaining MT=5 as a threshold reaction, with no discontinuity in the cross section. Let me stress this point: at each step in unfolding the remaining MT=5 starts at 0 cross section; there is never a non-physical discontinuity.

U-235 ENDF/B-VIII

The one example that I will use is probably the most important isotope in any data file designed to handle nuclear fission problems, namely U-235. Let me start by stressing that this is an excellent evaluation that performs well in many applications. This evaluation is based on using MT=5 "I don't know" down to 1.0d-5 eV. If this does not cause you and your codes any problems please continue to use it; what I present here need not concern you. Unfortunately, I, or rather my codes, are having a problem so I present here an alternative form, post-unfolding that solves my problems.

Below we see the major ENDF/B-VIII U235 cross sections. Here we can see that MT=5 (n, anything) at lower energies is very small compared to the other cross sections. At 1.e-5 eV it is about 3,000,000 less than the total. At 1 MeV it is about 10,000,000 less than the total. Only at high energy does MT=5 become significant. Below the MeV range MT=5 it is very simple: we will see that it is only a part of (n, a); hardly a complex reaction. This is strictly the evaluator's decision, but it is worth mentioning that this (n, a) is so small that through all earlier versions of ENDF/B it has been omitted; in the evaluator's judgement it is not important in engineering applications.



Here, rather than ignoring it I will show how easy it is to unfold cross sections and limit MT=5 to start in the MeV range, or at such a high energy it can be ignored; again, the evaluator's decision.

What is Defined in MF=6/MT=5

Below we see that MF=6/MT=5 defines all light particles and isotopes resulting from the cross section defined in MF=3/MT=5. Here we will see a big difference between what the evaluators consider the **BEST physics** and what I consider the **BEST engineering**. For charged particle reactions physics tells us that there will be tunneling through the Coulomb barrier, so there is no hard and fast threshold. The evaluators chose to attempt to include this effect in their **BEST physics evaluation** by extending their last real energy point directly to 1.0e-5 eV with a zero cross section there; hence the somewhat strange looking lines across the below figuure. What was hard to see in the below plot YELLOW on white background is an important ERROR. U235 (n, alpha) Th232 should extend down to 1.0e-5 eV as 1.0 (unity); for some reason the BEST physics has it start at 120 keV?



In contrast because the tunneling is such a tiny effects added onto a tiny cross section, I judge that for my **BEST engineering evaluation** I can ignore the tunneling. Next, ENDF cross sections are defined in ENDF-102 to be zero outside their defined/tabulate range, but users often are not aware of this. So, I have added zero cross section points at the beginning of each curve. I also corrected Th232 to extend down to 1.0e-5 eV. In the above figure you can see that the evaluators in their **BEST physics** consider complex enough to require MT=5 all the way down to 1.e-5 eV. With my **BEST engineering** we will see that it is very simple, nothing more than a part of (n, alpha) up to the MeV range, which does not require MT=5, and instead it can be uniquely defined by unfolding.

Light Particles

The current ENDF/B-VIII U235 evaluation includes in MF=6/MT=5 details of all light particles emitted in the collective MF=3/MT=5 "I do not know". Here are two different views of exactly the same data using linear and log scaling for the Y axis, From these plots we can see that,

- 1) Below about 15 MeV every reaction emits 1 alpha particle (2-He-4), i.e., (n, alpha....)
- 2) Below about 1 MeV only alpha particles (2-He-4) are emitted, i.e., only (n, alpha)
- 3) Below about 10 MeV only neutrons and 1 alpha particles (2-He-4) are emitted, i.e., a mix of (n, alpha) and (n, n' alpha)
- Between about 1 and 6 MeV neutron multiplicity is about 1/2, indicating a mix of (n, alpha) (0 neutrons) and (n, n' alpha) (1 neutron)
- 5) Between about 7 and 15 MeV neutron multiplicity is close to 2, indicating almost pure (n, 2n alpha); by then (n, alpha) and (n, n' alpha) have decreased significantly.

Based on these results combined with the list of isotopes produced included in MF=6/MT=5, the three dominant reactions up to about 15 MeV, are U235 to Th232 (n, alpha), Th231 (n, n' alpha) and Th230 (n, 2n alpha).



Light Particles and Isotopes

When we separate light particles and isotopes we can clearly see, For light particles,

1) Below about 1 MeV there is only (n, alpha).

2) Below about 10 to 15 MeV there is only (n, alpha), (n, n' alpha) and (n, 2n alpha) For isotopes,

1) Below about 1 MeV there is only Th-232.

2) Below about 10 to 15 MeV there is only Th-232, Th-231 and Th-230

Combining these results, we have a complete one-to-one match for three reactions that we can clearly see and unfold.

- 1) U-235 (n, alpha) Th-232
- 2) U-235 (n, n' alpha) Th-231
- 3) U-235 (n, 2n alpha) Th-230

Let us again give the evaluators credit for putting together this material in their **BEST physics** evaluation. For example, there are a multitude of reactions that potentially could lead from U-235 to these isotopes, but the evaluators did a great job putting together all of these results in MF6/MT5 so that we can see that below 10 MeV there are no other combinations of light particles emitted and isotopes produced. This allows me to produce a **BEST engineering** evaluation to unfold: MT=849 (n, alpha) continuum, MT=22 (n, n' alpha), MT=28 (n, 2n alpha), and move the start of MT=5 "I do not know" from 1.0e-5 eV to above 10 MeV.



Unfolding the Cross Sections

We now have the MF=3/MT=5 cross section in barns, and the isotope normalized production probabilities from MF=6/MT=5. The cross sections for the three reactions, MT=849, 22, and 28 are merely the product of the MF=3 cross sections and MF=6 probabilities. If I naively merely use the current Th232, Th231 and The230 as my first approximation for (n, alpha), (n, n' alpha) and (n, 2n alpha) we are left with the below probabilities. The remaining MT=5 "I do not know" would have a threshold at 10 MeV. In the second plot below, I have multiplied the probabilities from MF=6 by the cross section from MF=3 to define my initial GUESS of unfolded cross sections.



Let me repeat, the above is my initial GUESS, that I used to introduce the idea of unfolding. I do again thank the evaluators for providing all of the details that they have in MF=6/MT=5. Without these details on both particle multiplicities and isotope probabilities, we would not be able to see beyond the point where the isotope productions overlap. This increases our confidence as to the shape of the "hidden" reactions. However, be warned that this initial guess is not what I expect for alpha emission, and I may be over-simplifying the results too far in energy. I expect these alpha producing reactions to peak and then decrease toward zero, not increase as I see in my initial guess; this initial guess still needs work, but hopefully are good enough to introduce you to unfolding.

Remainder: New MT5

After removing the three easiest reactions the below figure shows the remaining MT=5 and all of the isotopes produced. In principle there are 12 isotopes, but 5 of these have a probability of 1.0e-7 or less (shown in **RED**) and I judge these can be ignored; they will never be seen in any **real engineering application**; these are the 5 **89-Ac** isotopes. Here we see the new MT=5 starts at 10 MeV. This is as far as I will go here, I leave it as an exercise for readers to unfold the next few reactions, or all of them. Here is a list of the remaining isotopes in ascending "threshold" order, and how many protons (p) and neutrons (n) needed to get from U-235 + n to this final product. To start, see if you can find the ENDF MT that corresponds to each isotope based on the needed p and n. For example, 1p 1n = (n, n' p); 1p 2n = (n, 2n p), etc. An obvious one is 0p 4n = (n, 4n). If you cannot find a defined MT, you have found a case where currently MT=5 is required, but you can report it to NNDC and see if they can define a new MT number.



VERY IMPORTANT: throughout this report I am assuming the MT=5 data in the current ENDF/B-VIII U235 is EXACT = **BEST physics** evaluation. The only exceptions being: 1) I corrected the Th232 probability, extended to 1.0e-5 eV, 2) I ignored charged particle tunneling; the original evaluation extended reaction down to zero at 1.0e-5 eV, and in my attempt at the **BEST engineering** evaluation I ignored tunneling and stopped each reaction at the lowest non-zero cross section energy for each reaction in the current evaluation. This tunneling effect in the current **BEST physics** evaluation produces the strange extensions we see in the second plot in this report, and the equally strange effect in the above plot where we see a sudden drop in cross sections; this is where I have defined the effective threshold for my **BEST engineering** evaluation. If I were actually doing an evaluation I would use more care in defining these effective thresholds, but this would have little effect on **engineering applications**; the extended probabilities are so small.

Defining the Secondary Distributions

Here is where we see the REALLY BIG difference between the **BEST physics** evaluation, which is the current ENDF/B-VIII U-235, and what I would propose as my **BEST engineering** evaluation. First, let me again complement the evaluators for providing all of the detailed information I need to unfold three reactions, e.g., we can see that the three reactions that I can easily unfold emit 0, 1 or 2 neutrons. **But unfortunately there is no information in the current ENDF/B-VIII evaluation in MF6/MT5 uniquely defining the secondary energy or angular distribution of individual secondary particles, such as each neutron; 0, 1 or 2** This is in line with ENDF-102 rules where it states that MT=5 cannot use MF=4 (directions) or MF=5 (secondary energy); it can only use MF=6, and in MF=6 no details are provided as to the secondary distributions of individual emitted particles, which is what we require for engineering problems for fission reactors.

Unfortunately using MT=5 "I do not know" in a **BEST physics evaluations** will not meet our needs to allow us to track secondary particles separately, as is required in any complete ENDF **BEST engineering evaluation**. I enquired about this point with the evaluators and was told they did not think it was possible to define the required secondary distributions. Here is the BIG difference: for an ENDF evaluation to meet the need that ENDF was designed "I do not know" just will not cut it; to be a complete **engineering evaluation** if we do not know ENDF data exactly **we MUST use our knowledge to provide our BEST GUESS**. That is what I have done for use with my codes; without providing the secondary particle information that my codes expect they can become confused and produce rubbish results - or worse - the mistakes may not be obvious to me, and I might believe that the rubbish results are correct.

So, what do I use to solve my secondary distribution problem? As Kipling wrote, therein lies another story, and it will have to wait for another day. Here I have only tried to introduce cross section unfolding to the point of showing how easy it is to use to unfold MF=3 cross sections, but not to the point of actually interfering with current evaluations. I will only state that in my case, to meet my needs, I need to define each secondary neutron and photon or else my processing and application code will become confused; sorry , these codes do not understand "I do not know".

Above I show my initial "guess" at unfolding based strictly on the contents of the current ENDF/B-VIII U235 MT=5 data in MF=3 and MF=6. Using the existing MF=6/MT=5 data I can easily identify and unfold three reactions from the MT=5 data and move its MT=5 threshold to 10 MeV. If you look at the above plots of the isotope and emitted particles you can see that unfolding can be used to identify more reactions and press the MT=5 threshold even higher. But we have already done enough as a brief introduction to unfolding.

Conclusion

Here I have attempted to show that MT=5 can easily be confined to as ENDF-102 currently states **COMPLEX REACTIONS AT HIGH ENERGY**; I will add hopefully above 20 MeV, so that it does not interfere with the traditional fission applications that ENDF was designed for. I have tried to stress the difference between a **BEST physics** evaluation where we need only uniquely define what we actually know, and are allowed to say "I do not now" for the rest, and a **BEST engineering** evaluation, where in order to be uniquely used in applications we MUST uniquely define all quantities; "I do not know" does cut it; when necessary we MUST provide our BEST GUESS. The one thing I do not have to GUESS is: **there ae no COMPLEX REACTIONS at low energy, so there is NEVER any NEED to contradict ENDF-102 and use MT=5 at low energy.**

The Future

After over 50 years of working with and whenever I can supporting the ENDF effort, I do fear for the future of ENDF. 50 years ago, CSEWG was composed of a balance between data producers and users, but **it was always driven by the needs of the users**. ENDF has been such a great success because the data providers and users all agreed to work together all using the common rules defined by ENDFD-102. Back then I think we all understood the difference between the BEST physics and the BEST engineering, and we agreed that for ENDF to meet its desired goal it was important that the final distributed release of **each version of ENDF only include the BEST engineering** evaluations; each of which was complete and as easy as possible to use in **engineering applications**.

What I am afraid of is that this agreement and goal have been lost, with a tendency to add progressively more BEST physics to ENDF, without regard for whether it can actually be used to meets the needs that ENDF are designed to meet: **AGAIN**, **THE NEEDS OF USERS IN ENGINEERING APLICATIONS**. To me the original pressing need for good data that we had 50 years were met by ENDF 20 years ago. Since then, there have definitely been incremental improvements toward the original goal. But I see progressively more effort being used to press ENDF into applications areas where it was never intended. I certainly have no objection to this, as long as it do not interfere with ENDF's original goal; interference that could lead to problems with the millions of dollars we have invested in codes to support our fission applications. To me introducing MT=5 (n, anything), which as far as my codes are concerned means "I do not know", which is o.k. for **BEST physics**, but it simply does not work for **BEST engineering**, and I fear it is only the tip of the iceberg that is shifting the balance away from meeting ENDF designed purpose: **Give engineers complete engineering evaluations that WE can use in OUR applications**.

My parting shot is that after over 50 years of using and in every way possible supporting ENDF I think it has more than adequately met it is initial goal, to support fission and fusion calculations, and it is time to stop trying to stretch it for use in other applications. I have no objection to applying

ENDF in other areas, but I fear that this is interfering with its initial objective; in my opinion MT=5 is but one example. Me thinks it is time to leave ENDF as it is and move on to GNDS, which seems to be the wave of the future. I suggest we start devoting more time, energy, and most importantly money to GNDS, in particular to developing the system of supporting codes that it will require.

Most important is my advice to you to not take this too seriously; enjoy life and remember you will never win a Noble Prize [6] for working on ENDF.

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[4] **EPICS2023: August 2023 Status Report**, IAEA-NDS-0242, by Dermott E. Cullen, Nuclear Data Center, IAEA, Vienna, Austria, August 2023

[5] **THESIS**: "Numerical Solution of the Linear Integral Boltzmann Equation", by Dermott E. Cullen Nuclear Science and Engineering, pp. 93-106, Vol. 53, Number 1, January 1974.

[6] **Noble Prize:** No that is not a typo; it is my attempt at humor. Unlike the more famous prize with a similar name, the Noble Prize is usually given each year to a farmer who is found to be **Out Standing in His Field.**

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