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Doppler Broadening and other Temperature Effects

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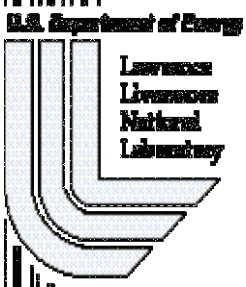

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DISCLAIMER

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Prologue

In this paper I attempt to document what I have learned and still remember about temperature effects, particularly Doppler broadening, on nuclear data, as it applies to ENDF formatted data. My focus is on the SIGMA1 method of Doppler broadening that I developed over 50 years ago. However, I do realize that there are currently many different methods used in computer codes, and I have tried to keep my discussion general as it applies to ALL of these methods. In particular, ALL of the MYTHS I describe below apply to all Doppler broadening methods: they all solve the parabolic diffusion equation in spherical geometry in (speed, reaction rate) versus temperature. These methods differ only in how the cross section is represented. So, at 85 years old here is what I still remember.

Overview

Over 50 years ago I published a paper entitled "Exact Doppler Broadening…" [1, 2]. I used what I considered at the time to be the provocative word "Exact", to see if anyone would rise to the occasion and question my claim. Unfortunately, so far nobody has, and what I call my SIGMA1 Method [3] has become THE standard method in many major ENDF processing codes, for Doppler broadening nuclear data in the ENDF format [4]. At the time, my "EXACT" claim was based on the model: 1) free atoms and 2) linearly interpolable tabulated ENDF formatted cross sections.

Since that time, I have learned from experience (mostly user feedback and code comparison) that my original method needs updates/corrections to correctly interpret all ENDF-102 data [4]. **I am now 85 years old, and I have been dealing with the problem of Doppler Broadening and learning about it for over 50 years. Here I will attempt to document what I have learned over these many years, in the hope that I can pass on this experience to the next generation, while I still can.**

Acknowledgements

First I must acknowledge many people who contributed to my efforts to assist in the development and continuing support of the ENDF systems, for the last 60 years. It takes a village, and we could not have reached the point where we are today without the coordinated work of Maurice Greene (AMPX), Chuck Weisbin (MINX), which later became Bob McFarlane (NJOY). Early on we all recognized that our codes are far too complicated to assume any one of them could get the right answer; **code comparison was essential.** Fortunately, this effort continues today in the work of Doro Wiarda (AMPX), and Wim Haeck (NJOY). Also, I must acknowledge the contributions of Jean-Christophe Sublet and S. Ganesan, who have continued to look over my shoulder and correct my mistakes

for many years. Lastly I thank Sol Pearlstein, the first head of NNDC and chairman of CSEWG. Sol more than any of us contributed to the success of ENDF by keeping us focused on the true objective: the ENDF Bible, ENDF-102 is not intended as a physics textbook; it is an engineering user's manual designed solely to help in nuclear engineering applications.

History 101

My first job after graduate school was at what became known as the National Nuclear Data Center (NNDC), Brookhaven National Laboratory. My doctoral thesis was on integral neutron transport theory, but at the time I realized that the biggest problem we faced in transport calculations was not the methods used, but rather the lack of accurate nuclear data. Without accurate data we were in a "garbage in – garbage out" situation. So, I decided to initially devote my time to improving our nuclear data; the timing seemed perfect because in 1965 Henry Honeck had just started the Evaluated Nuclear Data File (ENDF) project at Brookhaven.

At the time there was no U.S. national nuclear data system. Henry based his ENDF system on the British UKNDL system. The idea was to create a computer independent, simple text based system (at the time an 80 column computer card format) that could easily be transmitted in a computer readable form between data users. It was assumed that data users could then translate from ENDF to their existing in-house nuclear data system, which was at the time differed from user to user.

My initial task as head of the computer section of NNDC, was to develop software tools to support the ENDF effort. Henry's idea for an exchange format for nuclear evaluated data led me to develop a similar system for the exchange of Experimentally Measured nuclear data (EXFOR – X4) that could be used by evaluators to create ENDF evaluation; X-4 still exists today in virtually the same form I created it, and it still seems to meet its need. I should mention that my view of ENDF differs from

Henry's in that I realized that before we released ENDF data to the general public for them to **process** for their individual applications, we at NNDC could further assist users by **pre-processing** ENDF data by performing common operations that all ENDF users would face, such as: reconstruct resonance data, linearize all tabulated data, Doppler broaden, etc. This led to my developing my **ENDF Pre-Processing codes**; today's latest release being PREPRO2023 [6].

My next task was to allow us to "see" the ENDF data. This involved linearizing and reconstructing cross sections and displaying them. The first public view of ENDF/B data was of ENDF/B-III data [11]; the earlier releases of ENDF/B were not publicly available, since they were restricted from public release to within the U.S. by the AEC, later DOE. The availability of this tabulated linearly interpolable ENDF/B cross sections (MF=3) gave me the idea to add Doppler broadening to our collection of ENDF support software, as part of PREPRO [6].

Doppler Broadening

Doppler broadening is extensively described from both the physics and mathematics viewpoint in references [12, 13]; here I will only briefly describe it. Initially to me this was merely a straightforward mathematics problem, to describe the cross sections in the **Lab** system, where we perform all of our application calculations, starting from ENDF cross section, which are ALL in the center-of-mass, or **stationary** target (0 Kelvin) system. The accuracy of the ENDF data was a big step toward improving our ability to accurately perform transport calculations, but unless we were interested only in designing refrigerators at 0 K (-273.6 C), we needed Doppler broadened data in the LAB system. As we will see below, there can be a BIG difference between the ENDF C-M cross sections, as distributed by NNDC, and LAB cross sections that we actually use in our applications.

The following is essentially copied from [13]. The integral form of the Doppler broadening equation that I started from is modelled as free atom target atoms in a normalized Maxwellian distribution, $p(\bar{V}_T)d\bar{V}_T$, and tabulated linearly interpolable ENDF data, $\sigma(V,T)$, in both C-M and LAB systems (i.e., ENDF input and output are both linearly interpolable).

Lab reactions = Relative reactions

$$R(V,T) = V\sigma(V,T) = \int_{[Vt;Vr>0]} R(V_r,0)p(\bar{V}_T)d\bar{V}_T = \int_{[Vt;Vr>0]} V_r\sigma(V_r,0)p(\bar{V}_T)d\bar{V}_T$$

Since $p(\bar{V}_T)d\bar{V}_T$ is a normalized distribution, it is obvious from this equation that if the reaction rate $V_r\sigma(V_r,0)$ is constant the broadened cross section $V\sigma(V,T)$ will also be constant, independent of temperature, regardless of the model, $p(\bar{V}_T)d\bar{V}_T$, used to describe the thermal motion of the target nuclei. **That is to say a 1/V cross section will be independent of temperature.** It has been demonstrated elsewhere that a 1/V cross section is the only cross section shape that is independent of temperature. Therefore, in all other cases we must consider Doppler broadening since we expect the laboratory (LAB) cross section to be temperature dependent. My solution to this equation using ENDF tabulated, linearly interpolable cross sections as both input (at T1) and output (at any higher T2) I called the SIGMA1 method [3].

About 50 years ago when I first wrote my SIGMA1 [3] code I gave copies to my good friends, Maurice Greene for his code AMPX, and Chuck Weisbin for his code MINX, that later became NJOY, managed by Bob MacFarlane. This allowed us to verify that all three codes (AMPX, MINX/NJOY, SIGMA1) could calculate the same Doppler Broadened cross sections. We assumed the job was well done and finished, so we all moved on to tackle other problems.

What we learned

It took a few years until my good friend S. Ganesan pointed out to me that we cannot define ALL cross sections in the ENDF format to be uniquely represented as free atom, linear interpolable cross sections. The exceptions being,

1) ENDF does not define the cross section below the lowest tabulated energy down to the zero energy limit of the Doppler Broadening equation. How the cross sections (reaction rate) are extended down to zero energy turns out to be very important in our applications, to maintain temperature independent 1/v capture and fission cross sections at low energy, e.g., thermal energy range. Also, ENDF does not define how to estimate the energy dependent cross section from the upper energy limit of the resolved region into the unresolved region average cross section included in ENDF tabulated data.

2) Based on ENDF-102 in the Unresolved Resonance Region we do not uniquely know energy dependent cross sections. ENDF only defines a distribution of Breit-Wigner widths and spacing. By 1970, we at NNDC decided that the only cross section we could tabulate in the unresolved ENDF format is the **application independent, unshielded average** cross section, which has appeared in every version of ENDF since then [11]. This unshielded average varies directly as resonance width, inversely as spacing, and most important, as **1/v, due to unshielded averaging**. I say most important because generally widths and spacing in this energy range vary little, if at all; this does not mean the cross section does not vary – far from it. As a result, the unresolved region cross sections will be 1/v (due to unshielded averaging); completely unrelated to the width and spacing interpolation law (if any). The result of the **unresolved unbroadened average cross section in ENDF formatted tabulated data will be independent of temperature.**

3) **WARNING –** the ENDF unresolved region **unshielded** average cross sections are independent of application, but for any given application the **shielded** cross section can be 10 times or more smaller than the unshielded value shown in plots of ENDF data – see the below U238 capture.
4) At low energy, the best model may not be free atom; it may be bound atom – I will not discuss this model in this report.

I should add here one limitation not included in my SIGMA1 code but later added by some users; **Doppler broadening applies to ALL reactions, and ALL energies.** Some users restricted use to 1) only elastic, capture, fission, 2) no threshold reactions, 3) reduced energy range, e.g., not beyond upper energy limit of resolved range, 4) maybe others. 50 years ago, these limitations may have been justified to minimize computer time. Today computers are so much faster that these restrictions are simply not needed or justified, and limit use of SIGMA1. For example, with these limitations you cannot produce the fusion (D,D) Doppler broadened data shown later in this report. **I STRONGLY SUGGEST ALL SIGMA1 METHOD USERS REMOVE THESE RESTRICTIONS.** In terms of computer running time or storage, today you have nothing to gain by restricting when and where this method is used.

Once I recognized these limitations, I updated my SIGMA1 code to explicitly handle points 1) and 2) within the ENDF format, and I added logic/coding to handle bound atom scattering in my other processing codes. I then notified the users of my original SIGMA1 code that I was aware of, and suggested they update their versions of the SIGMA1 codes. These updated/corrections were documented in textbooks as long ago as 1986 [12], and more recently in 2010 [13]; i.e., almost 40 years ago.

Unfortunately, by the time I recognized these limitations to my original SIGMA1 method, the method was so deeply embedded in many

producing codes as a problem solved, even today decades later these codes may still include the limitations of my original SIGMA1 method.

A MAJOR purpose of these report is to inform all users of the limitations and to identify the MYTHS about Doppler Broadening – we cannot re-do history, but hopefully we have learned and can avoid repeating these mistakes.

Myth Busters

Here I will attempt to recognize ALL, or as many as I can remember, of the MYTHS that I have learned over the last 50 years of dealing with free atom Doppler broadening,

#1: **Nuclear Cross Sections are NOT temperature dependent**. In the relative, or center-of-mass (C-M), system, at any given relative speed between a particle (neutron) and target atom the cross section is independent of temperature. However, we perform our transport calculations in the laboratory (LAB) system; what we call Doppler broadening is due to simple mechanics, not any complicated nuclear physics.

In the free atom model the atoms of the target are moving about in an isotropic Maxwellian distribution. It is the motion of the target atoms relative to the incident neutron than changes the relative speed between the incident projectile and the target. This shift may seem small to you, but even at room temperature of 293.6 Kevlin (my apologies: in the text of this report and plots for simplicity I round this to 300 K), about 25 milli-eV average energy, this is enough to shift a neutron from one side of a narrow U238 milli-eV wide capture resonance, to the peak, or all the way to the other side (up or down) of the resonance. This frame of reference dependence should not come as a surprise to anyone. It is the same reason that until relatively recently in history mankind assumed the Sun rotates

around the Earth; it is what we see every day from sunrise to sunset. This was such a radical idea that when it was initially proposed some people were burned at the stake as heretics for proposing it. I can only hope that my explaining Doppler broadening here does not result in a similar fate for me.

#2: **Doppler Broadening Smooths Reaction Rate, NOT cross sections**. This is a VERY IMPORTANT point. Cross Section (barns) is not physically observable, whereas reactions are; e.g., reactions per second. What the Doppler Broadening equation attempts to do is define the LAB system REACTION RATE (v*cross section) to be identical to the center-of-mass REACTION RATE.

In our nuclear engineering applications, the difference is crucial. Far too many textbooks when they describe Doppler Broadening somehow lose the correct REACTION RATE relationship and end up with an equation that SMOOTHS cross section, rather than reaction rate, **which is simply WRONG for use in many of our applications..**

SMOTHNG REACTION RATE means that any reaction rate (v*cross section) that is smooth, will be TEMPERATURE INDEPENDENT. Or, in terms of cross section a 1/v cross section means a constant smooth REACTION RATE, so **a 1/v cross section be INDEPENDENT OF TEMPERATURE**. This is crucially important in our applications because low energy capture and fission cross sections tend to be /1/v, and therefore they tend to be independent of temperature. The same is true of the application independent unshielded cross section in the unresolved energy range.

#3: **Below the lowest tabulated ENDF energy (traditionally 1.0e-5 eV) we do not know the cross section,** so we obviously cannot uniquely define it all the way down to 0 energy, as required by my SIGMA1 method. However, based on point #2, above, we can extend the capture

and fission cross section as 1/v, i.e., A CONSTANT REACTION RATE, which will strongly tend to make them temperature INDEPENDENT.

Here the elastic cross section tends to be constant, so its reaction rate varies linearly as v, and below its lowest tabulated value it approaches zero, and it is so small that it does not matter how we extend it to 0 energy. Also, in "bootstrapping" cross sections the initial elastic, and all lower limits must be 1/v. **SIGMA1 now extend ALL reaction rates below their lowest tabulated value as a CONSTANT REACTION RATE.** This point is discussed, and results are shown in detail below.

#4: **In the ENDF UNRESOLVED RESONANCE REGION we do not uniquely know energy dependent cross sections**. As defined in ENDF-102 the entire UNRESOLVED RESONANCE REGION is only defined by distributions of resonance widths and spacings; we cannot uniquely define tabulated linearly interpolable cross sections required by my SIGMA1 method.

I must take the blame for making this fact less obvious to ENDF users, who "view" ENDF cross sections. When I worked at NNDC, BNL, just as ENDF was starting (1967-72), one of our first problems was to develop codes to view ENDF data. But since we do not uniquely know the UNRESOLVED resonance region cross section the question was how to include it in our tables of tabulated cross sections, to "view" the data. **We decided to tabulate only the application independent, unshielded average cross section.** For over 50 years this is still what appears on our plots of tabulated so called "energy dependent" ENDF cross sections.

This turned out to be a lucky choice (I admit luck, not skill). With the ENDF definition of unresolved resonance width and spacings the most prominent traditional definition is a so called picket fence of constant widths and spacings. Using ENDF-102 definitions these constant widths

and spacing produces an average, unshielded 1/v cross section; **CONSTANT REACTIONS = TEMPERATURE INDEPENDENT.**

There is an ERROR in ENDF-102 [1]; the interpolation law included with the unresolved widths and spacing, as with all tabulated ENDF data, refers to the widths and spacings. **ENDF-102 now ERRORNEOUSLY states it applies to the cross section.** As explained above, this is NONSENSE.

Bottom Line: **SIGMA1 now assumes the entire UNRESOLVED RESONANCE REGION is TEMPERATURE INDEPENDENT equal to the unshielded average usually 1/v cross section we have been outputting with our tabulated ENDF data for over 50 years.** But be WARNED: the actual **shielded** average unresolved cross section in any given application can be a decade (10 times) smaller than the **unshielded** value shown, due to self-shielding [14].

#5: **Reactions Threshold can change due to Doppler broadening**. Exactly the same as in the case of resonances, thermal motion of atoms can shift a neutron's Lab speed from below a threshold to a center-of-mass speed above it. For fission applications with a milli-eV-like temperature this will generally be a minor effect that can be ignored. But for astrophysical applications it can be very important. As I will illustrate below, for keV-like temperatures reactions with thresholds in the center-of-mass system, may end up not having any threshold in the LAB system. Below I will illustrate this effect for an important fusion reaction. One minor point: a neutron exactly at the threshold of an inelastic threshold will not end piling up at 0 energy; it will end up in a Maxwellian distribution, that my TART [7] Monte Carlo code correctly calculates.

#6: **Doppler broadening applies to ALL reactions at ALL energies.** Not a limitation of my SIGMA1 method but added by some users. No longer needed – **I SUGGEST YOU REMOVE THESE LIMITATIONS**. But be warned: any cross section that extends down in energy to the resonance

region should be correlated to the resonances. This applies to the high energy extension of ENDF to 100 MeV, where MT=5 (n, anything) was created specifically to handle **complex reactions at high energy**. Instead, it is now being misused to handle simple reactions at the lowest tabulated ENDF energy and show no correlation to the resonance region.

BE WARNED: failure to "see" correlations usually indicates misuse of a nuclear model code, which is not actually designed to model/include resonances. I mention this here because these uncorrelated data will show little, if any, Doppler broadening.

#7: **The Doppler Broadening equation that SIGMA1 solves is the DIFFUSION EQUATIION in spherical (reaction rate, speed) coordinates vs. temperature.** You may have used this to mathematically solve the same diffusion equation for heat (temperature, space) vs. time, or even neutron diffusion (flux, space) vs. time.

The diffusion equation has well known mathematical and physics properties. First, the good news **mathematically it an initial value parabolic equation,** which means we can start at any initial temperature and **"bootstrap" up to any higher temperature**. I use this property to save an incredible amount of computer time to create temperature dependent ENDF data libraries [5], tabulated at temperatures: 0 to 300, 300 to 600, etc. – the biggest step in terms of reducing the number of ENDF energy points involved is the step from temperature 0 to 300 (actually 293.6) Kelvin.

#8: **The initial value diffusion equation involves dT rather than T. In my SIGMA1 method I use the integral form of the diffusion equation, where it is clear that we cannot use this integral equation to UNBROADEN cross sections.**

Mathematically is it obvious we cannot use this equation to unbroaden cross sections; the integral equation makes no sense for a Maxwellian with a negative temperature (positive exponential). **Physically** this would be a violation of the second law of thermal-dynamics, trying to decease lethargy, or creating order out of chaos.

This is an argument I have had with any number of people over the last 50 years. To people who **use the differential form of the diffusion equation** it is not at all obvious we cannot UNIQUELY unbroaden. In fact, you can start with any set of observed resonances at any temperature T1 and mechanically "unbroaden" them to a lower T2. This only poorly approximates the resonances you uniquely define to start with at T1 and cannot locate/separate overlapping resonances. This does not result in a UNIQUE solution at the lower T2. Because at the lower T2 there can be an infinity number of resonances that are too narrow or small to be observed at the higher temperature T1 – see the U238 capture cross sections below comparing 0 and 300 K cross sections; do you think you can uniquely define the 0 K data starting from the 300 K we see here. **If you use the integral form of the diffusion equation, as we do in my SIGMA1 method, it is obvious that the Exponential in the Maxwellian is NONSENE for dT negative.**

In summary,

Unique higher T (positive dT) results: Starting with any initial temperature the diffusion you can UNIQUELY broaden to any higher temperature; i.e., "bootstrapping" works = my SIGMA1 method.

Non-Unique lower T r(negative dT) results: If you have a room temperature measurement of resonances, you can **mechanically use the differential form of the diffusion equation** to approximate what the distribution looks like at 0 Kelvin; this is needed for use in ENDF evaluations. But this will not improve your knowledge (reduce lethargy); it will merely produce one of the infinity of distributions that can be

broadened to reproduce your room temperature measurement. In addition, CAVEAT EMPTOR – be WARNED this unbroaden is VERY NUMERICALLY UNSTABLE and can produce nonsense results.

Summary of ERRORS in my Original EXACT Method

In summary my 1970s version of so called EXACT DOPPLER BROADENING had the following ERRORS, all of which were corrected in textbooks almost 40 years ago [12, 13] and are now correct in the current 2023 version of SIGMA1 [6]. The correct interpretation include,

1) Extension of REACTION RATE (not cross section) beyond tabulated ranges (to 0 eV and beyond upper resolved limit).
2) Copy UNSHIELDED UNRESOLVED AVERAGES (temperature independent).
3) Allow MOVING REACTION THRESHOLDS
4) Broaden ALL reactions at ALL energies (a user added restrictions).

Before and After

The above points describe Doppler broadening, which is an effect due to the cross sections encountered in the LAB system **before a reaction.** All of these effects are now included in the latest version of my SIGMA1 code [6]. Thermal motion also has effects that we "see" after a reaction.

When a neutron scatters from a moving target it can UNSCATTER. At fission reactor temperatures of milli-eV you might think this effect is negligible, but U238 capture resonances can be milli-eV wide and isolated, so that even a small shift in energy can result in shifting a neutron from below any given resonance before a collision to the peak or to above the resonance after the collision, i.e., the neutron may have to pass a given resonance more than once. Also, inelastic scatters near the threshold will not result in a near zero energy secondary neutron, but rather a thermal Maxwellian due to motion of the target nuclei.

These "after the event" temperature effects are NOT included in my SIGMA1 method of Doppler broadening, but they are included in my TART [7] Monte Carlo transport code, using my THERMAL [8] routine. I was surprised at how high in energy this effect is important [9, 10].

Limitations of ENDF

What I have described above as Doppler broadening ONLY APPLIES to the OFFICIAL ENDF-102 defined format for tabulated cross sections in MF=3. MF=2 may be used to reconstruct the cross sections in the resonance regions. After reconstruction MF=2 is also needed to define the resolved and unresolved resonance regions to correctly use my SIGMA1 method. In particular note that my method of Doppler broadening only applies to cross sections (MF=3): it does not apply to transforming angular or energy distributions from C-M to LAB **if they are correlated to cross sections resonances**; the related cross sections MUST be smoothly varying with incident energy. Also note, MT=251, average scattering cosine in the LAB – MUST be defined in the LAB system; there is no ENDF-102 option to define this in the C-M system, as some evaluators have done; WARNING – this is an ERROR.

When Henry Honeck designed ENDF he originally designed it as a computer independent, simple text format, that could easily be exchanged between users/laboratories. It was assumed that once users received the data they could then translate it to their existing IN-HOUSE nuclear data system. While working at NNDC I used the same principles to design the EXFOR (X-4) format to exchange experimental data between users/laboratories; this data could be used by ENDF evaluators.

In the 1960s while at the NNDC, BNL I realized that we could help users by performing a few standard operations before distributing ENDF data to users who could then perform IN-HOUSE processing. This included:

1) linearizing the data, 2) reconstructing resonance cross sections, 3) Doppler broadening, etc. This is the origin of my ENDF Pre-processing codes, now named PREPRO [6]. The hope was that users could start their IN-HOUSE processing taking advantage of this pre-processed data.

Things did not work out exactly as I had hoped/planned. Today NNDC distributes the original ENDF evaluations from the evaluators; the latest being ENDF-VIII.1. Without any financial support I have continued to try to help by maintaining my PREPRO codes; the latest being PREPRO2023 [6], and by PRE-PROCESSING this data into POINT data; the latest being POINT2025 [5]. **What is important to understand is that my PREPRO codes, including SIGMA1, for Doppler broadening, are designed to work with the basic, complete ENDF evaluations distributed by NNDC.** Unfortunately, these complete ENDF evaluations distributed by NDC are not necessarily the same as the IN-HOUSE systems and formats used at many locations.

What did not work out exactly as I had hoped is that the IN-HOUSE and processed data produced by users is not the complete ENDF evaluations distributed by NNDC. For example, the ORNL (AMPX), LANL (ACE) and LLNL (ENDL) formats do not include a definition of the resonance region, so they cannot automatically define the energy range of the unresolved resonance region, as required with my SIGMA1 method [6].

Fortunately, these codes do now correctly extend the REACTION RATE down to zero energy as constant. Unfortunately, in a recent comparison of Doppler broadening codes I discovered that several **newer codes** are still using the ERRORS from my original method, in particular extending cross section, rather than reaction rate below the tabulated range. **This can result in ERRONEOUS DANGERUS RESULTS, where capture and fission appear to decrease with temperature = a safety hazard.**

To my knowledge, except for my SIGMA1 code none of these other codes account for shift in reaction thresholds with temperature or upscatter due to thermal motion. Sorry to have to mention that based on discussions with processing code designers, they admitted they had no idea how to include this effect in secondary distributions (angular and energy), so they decided to ignore this effect. Note, this decision was made in nuclear processing codes and usually the codes that actually use the data are not aware of these limitations in the data they have been presented to use.

Since I love puns I like to joke that as a result these IN-HOUSE processing systems are producing OUT-HOUSE processed data ready for use in unsuspecting application codes = **CAVEAT EMPTOR!!!**

BEWARE of Reich-Moore Results

First the Good News: Adding Reich-Moore (R-M) Cross Sections to ENDF, MF=2 (resonances) and derived MF=3 (derived cross sections) was a big improvement for ENDF cross sections. Unfortunately, the bad news is that R-M secondary information is being misused by evaluators. Today ALL distributed ENDF data is identified as being at 0 Kelvin temperature (-273.6 C), which means ALL of the R-M results are in the center-of-mass system, and for our use MUST be translated to the LAB system, in which we perform our applications. This is not a problem for the MF=2 and 3 cross sections, using resonance reconstruction and the Doppler broadening and other temperature dependent effects described in this report.

However, it is a problem for secondary distributions (angular and energy). To my knowledge none of our code, including my own PREPRO codes, can convert secondary distributions from **C-M to LAB IF THEY ARE CORRELATED TO CROSS SECTION RESONANCES.** In particular I will first mention, ENDF MT=251 = the Average Scattering Cosine in the **LAB** system.

Let me repeat this – **IN THE LAB SYSTEM**. There is no ENDF option to convert from R-M center-of-mass to LAB. In the center-of-mass system we know there is an asymmetric correlation between scatter cosine and resonances, increasing on one side of a resonance and decreasing on the other. But we have known since I was in graduate school in the 1960s that this asymmetry cancels out and disappears in the transformation from center-of-mass to LAB. So that **for the entire almost 60 year history of ENDF MT=251 in the LAB was correctly defined as smoothly varying, uncorrelated to any resonances.** This is no longer true in ENF/B-VIII.1; today's evaluations do not seem to understand the important difference, and ERRONEOUSLY include R-M CM data in MT=251, which is explicitly defined as ….IN THE LAB.

More serious ENDF-102 R-M MF=2 parameters now include an option to indicate that R-M angular distributions can be used. Sorry to have to say this so forcefully: **NONSENSE. I repeat none of our codes can convert angular distributions from C-M to LAB if they are correlated to resonances.** AND, more important, we should not have to, because any C-M to LAB Doppler broadening cancels out the C-M asymmetry; PLEASE evaluators do not use this option to present ERRONEOUS data.

When I tried to report this problem to NNDC as what I consider to be traditional users constructive criticism (feedback) I was told all of our codes can convert angular distributions from C-M to LAB, as my LEGEND [6], and this was not be problem. They could not understand that all of our codes **DO NOT INCLUDE CORRELATION TO RESONANCE, for any secondary neutron information.**

In Summary: We cannot use R-M secondary information in the C-M – PLEASE DO NOT INCLUDE IT IN ENDF evaluations. More

importantly, this data is not needed: for secondary angle and energy distributions C-M resonance effects disappear when CORRECTLY translated to LAB data, in which we use it.

Where ENDF is Today

Since ENDF started at NNDC, BNL 60 years ago, what has made it such a GREAT success was the agreement by everyone = producers, processors, users – to strictly obey the ENDF-102 rules and definitions defined by Henry Honeck and obey KISS = Keep It Short & Simple. Back then there was a close bond between data evaluators and users testing the data and supplying feedback = constructive criticism. The agreed focus was on: **ONLY INCLUDE WHAT IS ABSOLUTELY NECESSARY FOR OUR FISSION/FUSION APPLICATIONS**. For almost 50 years strict focus on the sole aim of ENDF resulted in what I feel is great nuclear data that meets all of my needs for my primary interest, Monte Carlo transport. I will mention again all of the supporting processing and applications code, which I estimate have cost more than a billion US dollars to develop and maintain - until recently these codes met all our needs.

Today the focus seems to have shifted from WHAT IS NEED IN APPLICATIONS to WHAT EVALUATORS ARE INTERESTED IN, to the point where the ENDF Bible ENDF-102 includes options that it states are not currently being used, but are included in case they are needed in the future by nuclear model codes – there is no such mention of what our applications may need, or any **mention/WARNING that by changing the ENDF-102 rules the billion dollars of supporting software may be put out of business, which has happened with ENDF/B-VIII.1.**

The Future of PREPRO

I hate to admit that after spending over 50 years trying to independently support the ENDF effort, with no official financial support or reward to

me, CSEWG and NNDC have managed to change the ENDF-102 format used in ENDF/B-VIII.1 to cause my PREPRO codes to crash and burn; VIII.0 was o.k., but VIII.1 is not. There are 558 evaluations included in ENDF/B-VIII.1, and only one, namely, Sr88, causes my codes to crash, because Sr88 uses an ENDF option that no data user needs, nor has any data user asked for it, and yet it has suddenly been added to ENDF-102; this was based strictly on the evaluators interests.

For all these years I have tried to be supportive, but I refuse to waste my time or energy trying to be supportive of what I consider to be unnecessary and frankly silly, so I have no intention of updating PPEPRO to handle the ENDF-102 extension used by 1 of 558 evaluations. When I informed the NNDC of this problem in what I considered to be constructive user feedback, that they had to choose between Sr88 and PREPRO, they chose Sr88. So be it; I will continue to maintain PREPRO for my own personal use for my TART Monte Carlo code [7], which I have done for ENDF/B-VIII.1 data in POINT2025 [5]. However, I can no longer distribute PREPRO to the public, since I admit these codes no longer work due to recent ENDF-102 format extensions. Note, that I have produced POINT data files [5] for each version of ENDF/B not because I think it is perfect, but rather so that we can all "see" the data and each judge for ourselves whether or not it meets the needs of our applications – if it does not meet your needs, PLEASE notify NNDC.

The bottom line is that after almost 60 years of development by our community and what I estimate to be over a billion dollars in salaries and computer times this leave ENDF with no codes that include all of the Doppler broadening and temperature effects described here. But not to worry you can still design "cold" 0 K refrigerators – just my sense of humor.

Based on many years of code comparisons I can recommend AMPX and NJOY; although they do not exactly agree with SIGMA1 Doppler broadening described in this report, they are close enough for most of our applications. Most important these codes, unlike PREPRO, which I personally maintained without any financial support, AMPX and NJOY have long terms support through National Labs; you can rely on them being here next year.

Examples of Doppler Broadening

In closing I present examples to illustrate the importance of Doppler broadening.

First I present results for **U238 capture**; a classic example of Doppler broadening resonances, Here I compare "cold", 0 Kelvin and "room temperature", 0 K and 300 K (actually 293.6 K = 20 C). The important points to note here include how high up in energy the effect of this relatively low temperature (293.7 K, 20 C, 25.3 milli-eV) extend; the narrow capture resonances up to 20 keV overlap and tend to disappear. Note, also the ENORMOUS discontinuity between the **energy dependent** cross sections in the resolved energy range and the **unshielded average** cross sections in the unresolved. Again, I will remind the reader that based on ENDF-102 resolved and unresolved definitions, and my decision over 50 years ago, to include the unshielded average cross section in the unresolved region **THIS DISCONTINUIY TO REAL AND WELL UNDERSTOOD.** I should add that this was true in earlier versions of ENDF evaluations but no longer seems to be understood in more recent evaluations; few newer evaluations even include an unresolved region, and of those that do it is obviously NOT the ENDF unshielded average smooth cross section that we traditionally expect = **CAVEAT EMPTOR!**

Next I present REACTION RATE and CROSS SECTION results for the lowest energy range - including thermal ranges. Here I present results for Elastic and Capture, and a light material, Hydrogen, and a heavy material, U238. Hopefully from these results the reader can appreciate the importance of extending the REACTION RATE, not CROSS SECTION, as constant below the tabulated energy range down to 0 energy.

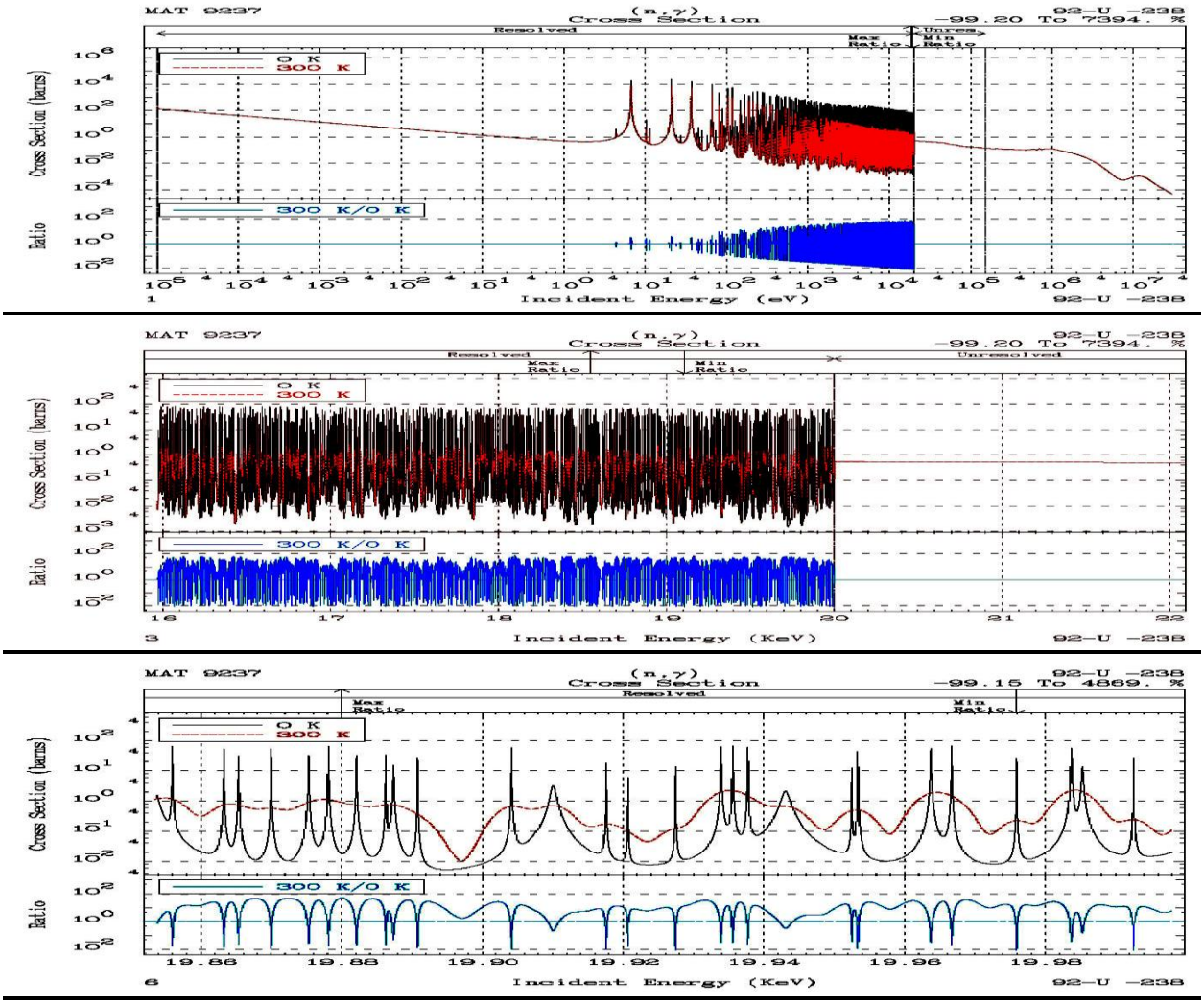
Lastly, I present a copy of a figure from [13] that illustrates the effect that high temperature has on cross sections that have a threshold in the C-M system but shift to lower and lower energy with increasing temperature and eventually at sufficiently high temperature there is no LAB threshold.

U-238 Capture: at 0 and 300 Kelvin

The below figures illustrate the enormous effect that Doppler Broadening has on the U238 Capture Cross Section at two temperatures: 0 and 300 Kelvin (room temperature). The below three figures show the U238 capture starting from an overview and zooming in to show details of the very narrow capture resonances near the upper limit of the RESOLVED resonance region at 20 keV.

First note the UNRESOLVED resonance region. This is what we expect from ENDF data; as explained above, this shows the UNSHIELDED average cross section. In a properly defined ENDF evaluation **the UNSOLVED REGION is smooth and INDEPENDENT of temperature.** Note, the expected discontinuity between the resolved **energy dependent** and unresolved **averages**.

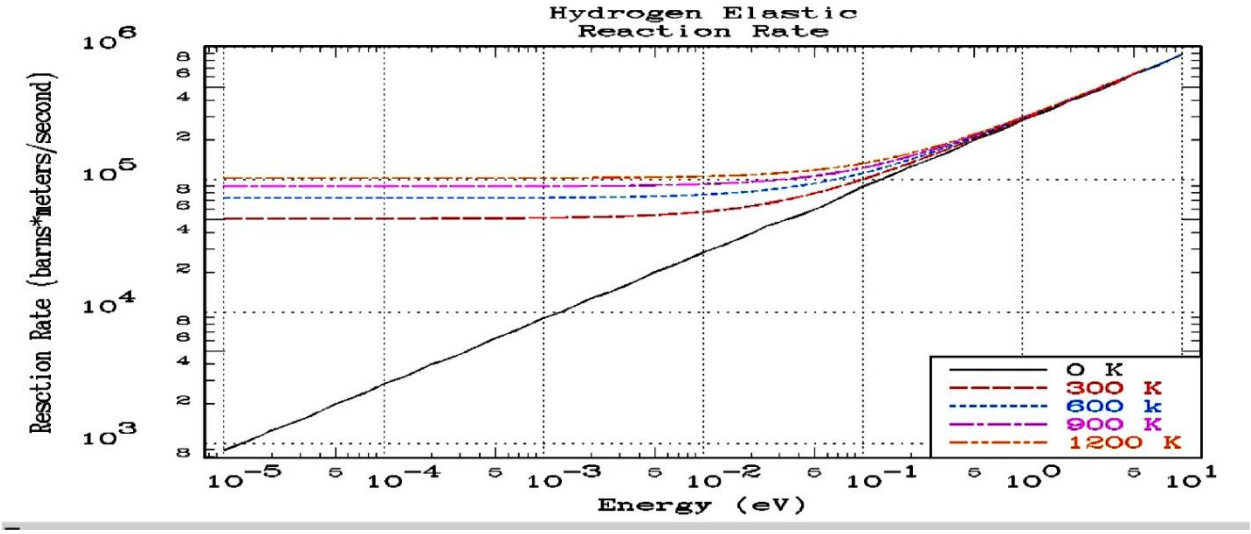
Next, **note the ENORMOUS effect that Doppler broadening has on these very narrow resonances**. The peak at resonances and valley between resonances change by almost **a factor of 100 – not 100% - a factor of 100!** The third plot shows that virtually all of the narrow resonances shown here up to 20 keV, disappear even at room temperature (300 K)

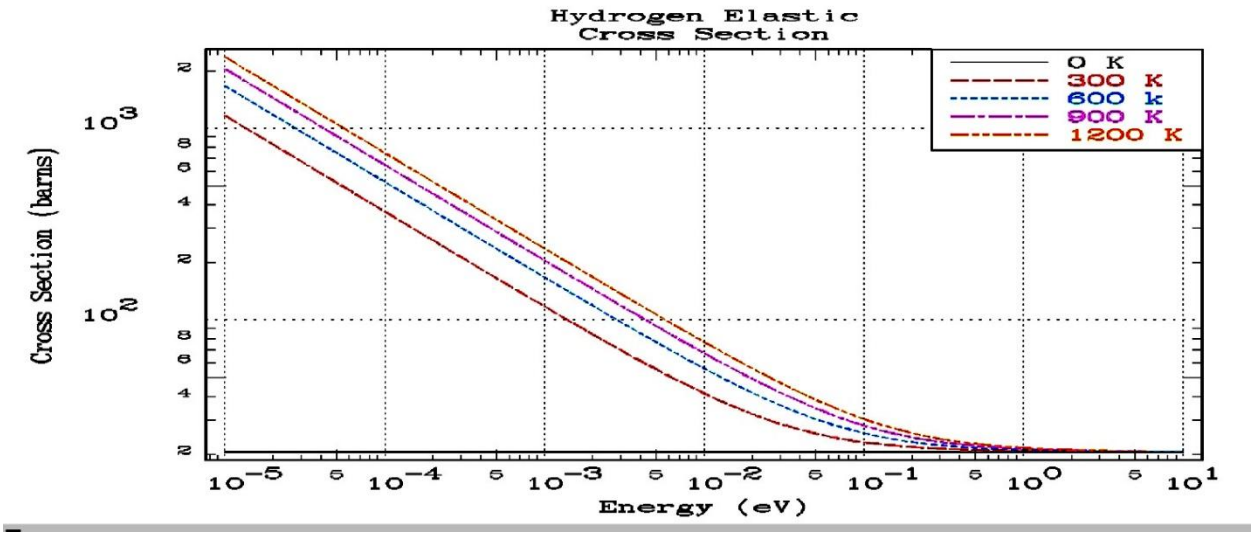


Hydrogen Elastic

Here we can see the Hydrogen Elastic **Reaction Rate**. At 0 Kelvin near low energies the reaction rate varies as V (neutron speed). As the temperature increases we see the Reaction Rate increase, filling in the "hole" near the origin" (V→ 0). Note that except for 0 Kelvin, the low energy limit approaches a constant, which it must in this spherical (speed, reaction rate) diffusion space. **Constant is what SIGMA1 assumes in extending the elastic Reaction Rate (not Cross Section) below the lowest tabulated energy (1.0d-5** eV) to "bootstrap" from one temperature to any higher temperature.

Next we can see the Hydrogen Elastic **Cross Section**, At 0 Kelvin at low energy it is constant. As the temperature increases we see the cross section increase. One of the BEST known cross sections is the free atom Hydrogen Elastic at thermal energy as 20 barns. **Even at this relatively low temperature (room temperature) Doppler broadening increases this to 30 barns; a 50 % increase. Hopefully, this shows the importance of Doppler broadening at low energy.**

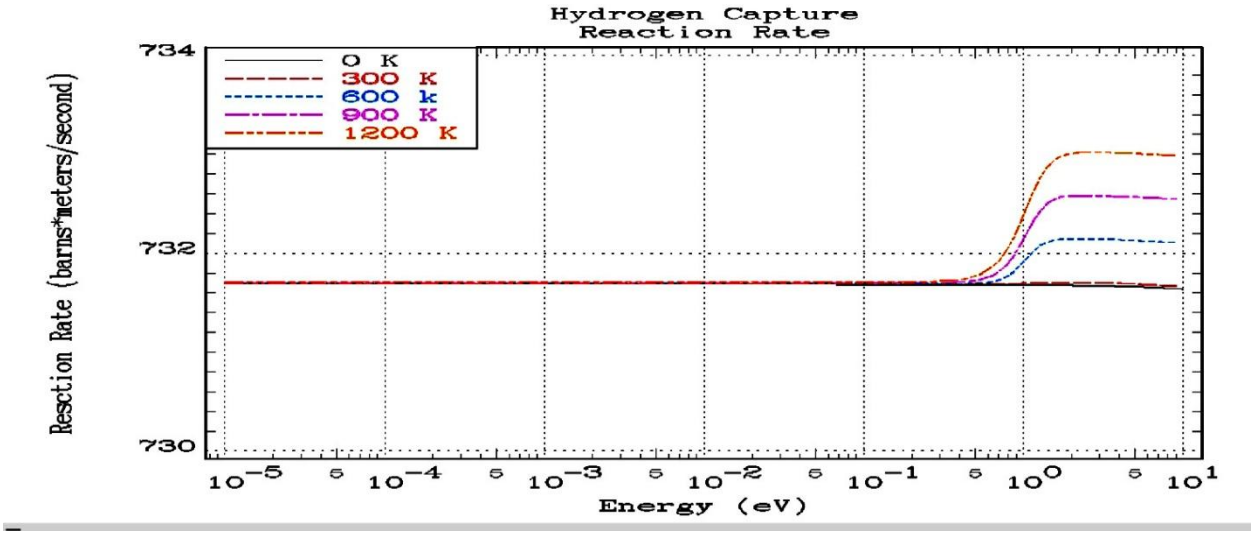


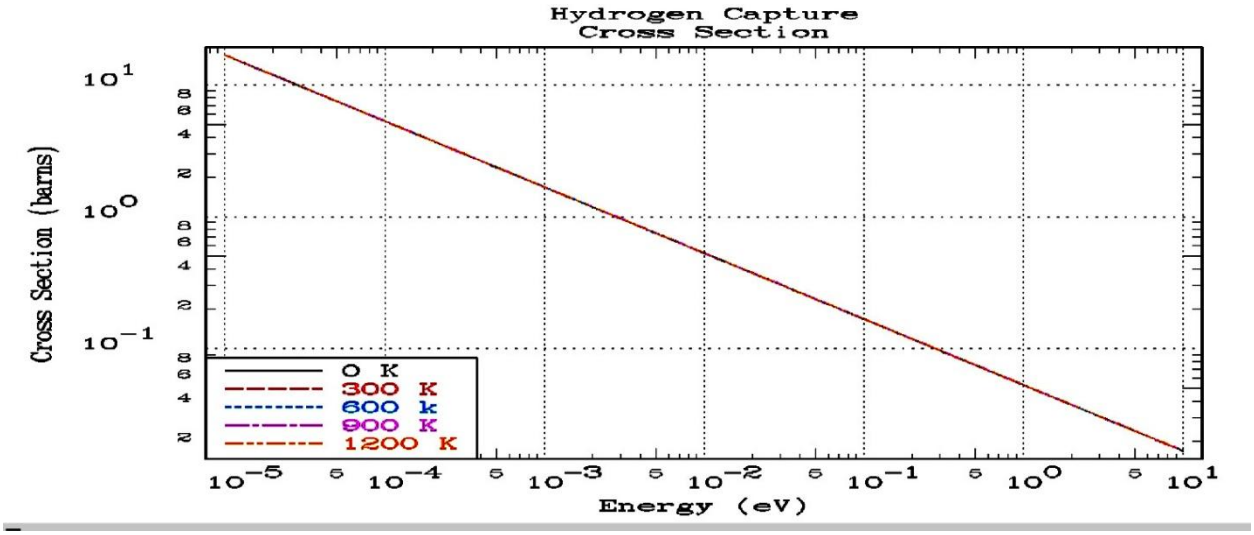


Hydrogen Capture

Here we can see the Hydrogen Capture **Reaction Rate**. At 0 Kelvin near low energy, it is constant. As the temperature increases since the Reaction Rate is already constant we see essentially no change below the eV energy range.

Next we can see the Hydrogen Capture **Cross Section**. At 0 Kelvin near low energy varies as 1/ V. **Since the Reaction Rate is constant, as the temperature increases we see virtually no change in the cross section. Hopefully, this illustrates the importance of extending the Reaction Rate (not the Cross Section) as CONSTANT below its lowest Tabulated energy (1.0d-5 eV).**

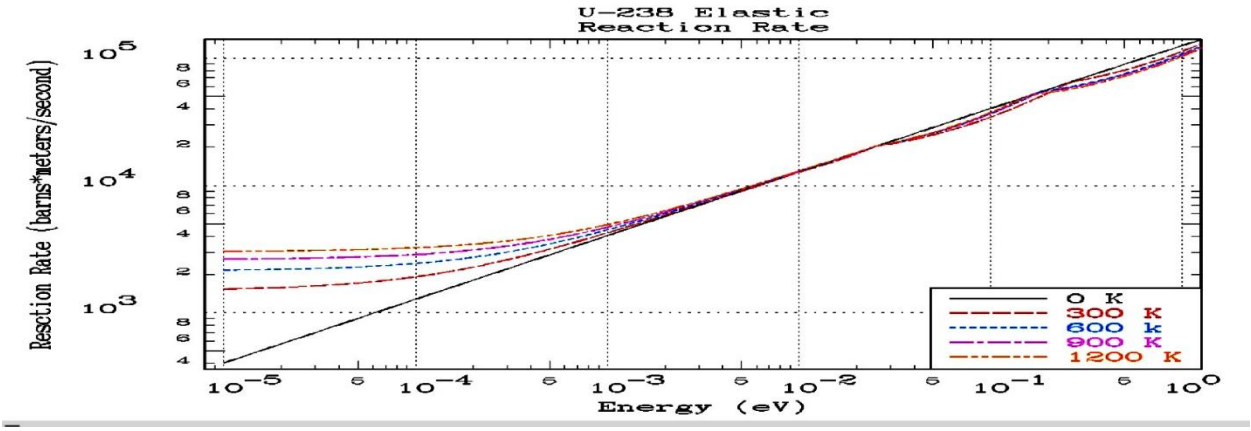


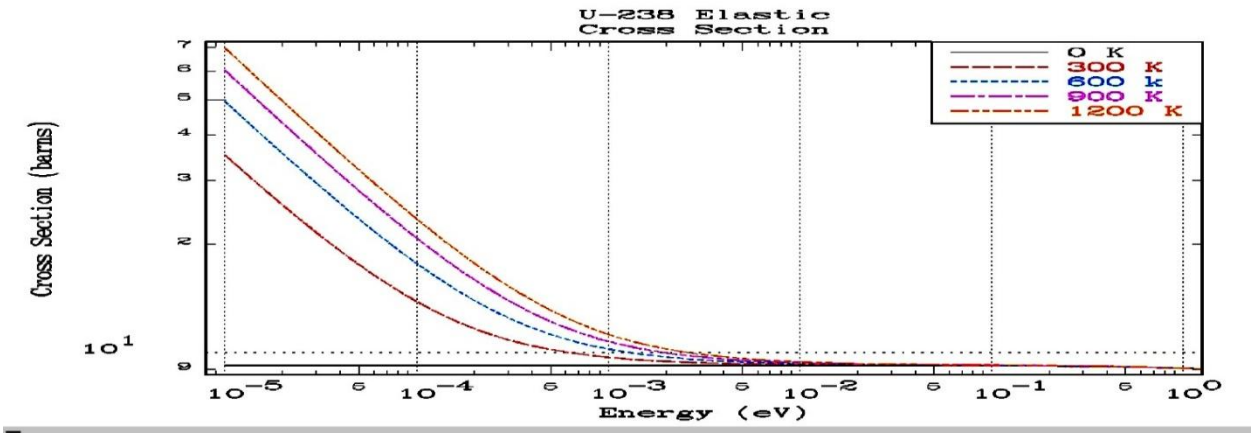


U238 Elastic

Here we can see the U238 Elastic **Reaction Rate**. This is similar to the Hydrogen Elastic Reaction Rate, in that at 0 Kelvin near low energies the reaction rate varies as V (neutron speed). As the temperature increases we see the Reaction Rate increase, filling the "hole" near origin" (V→ 0). The difference from Hydrogen is that for the same temperature defined by energy, $E = m*V^2/2$, the speed (V) of the U238 atoms will be lower by sqrt(m) ~ sqrt(A), A=238; sqrt(A) ~ 15. So that the broadened reaction rate (and cross section) are shifted downwards in energy, by over an order of magnitude. As a result, it does not have as large an effect on the thermal cross section as the 50% we saw for Hydrogen. As with the hydrogen, except for 0 Kelvin, the low energy limit approaches a constant, which it must in this spherical (speed, reaction rate) diffusion space. **Constant is what SIGMA1 assumes in extending the elastic Reaction Rate (not Cross Section) below the lowest tabulated energy (1.0d-5** eV) to "bootstrap" from one temperature to any higher temperature.

Next we can see the U238 Elastic **Cross Section**, At 0 Kelvin at low energy it is constant. As the temperature increases we see the cross section increase. Again, compared to the Hydrogen Elastic cross section the U238 increase is shifted to lower energy, and has a much smaller effect at thermal energy. **Comparing the H and U238 elastic we can see that in the low neutron energy range Doppler broadening has a larger effect on light (low A) materials.**

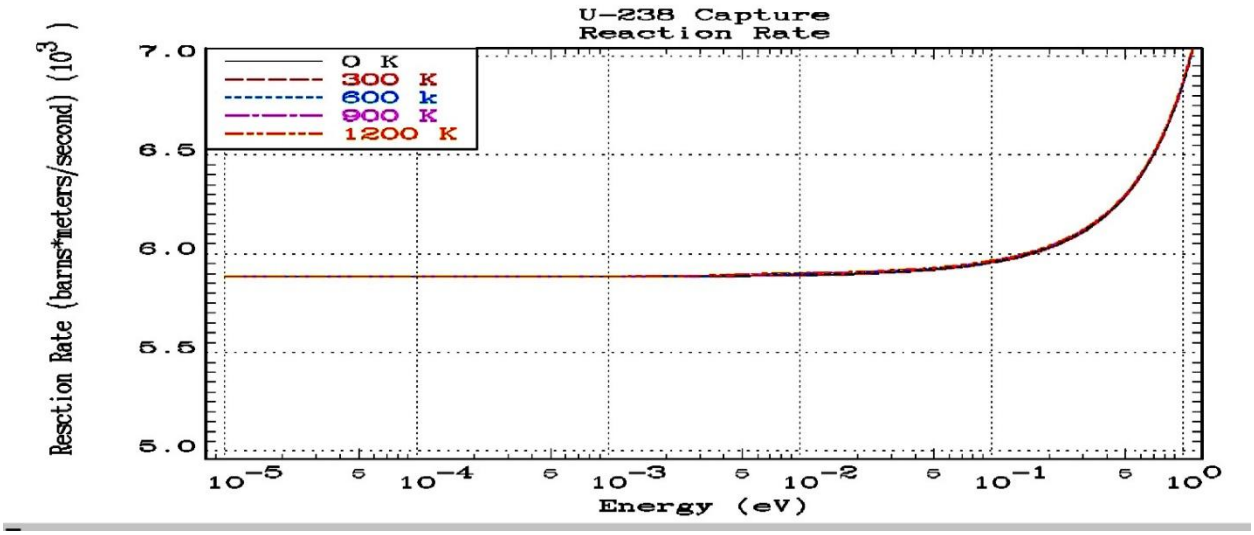


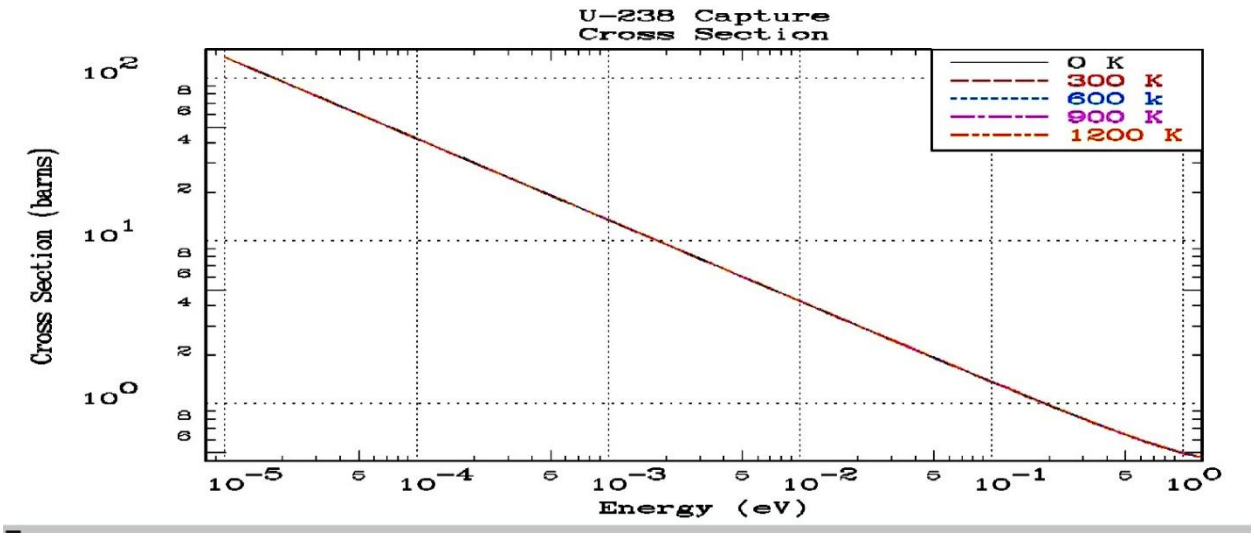


U238 Capture

Here we can see the U238 Capture **Reaction Rate**. Similar to the Hydrogen Capture, at 0 Kelvin near low energy it is constant. As the temperature increases, since the Reaction Rate is already constant, we see essentially no change below the eV energy range.

Next we can see the U238 Capture **Cross Section**. Similar to the Hydrogen Capture at 0 Kelvin near low energy it varies as 1/ V. **Since the Reaction Rate is constant, as the temperature increases we see virtually no change in the cross section. Hopefully, this illustrates the importance of extending the Reaction Rate (not the Cross Section) as CONSTANT below its lowest Tabulated energy (1.0d-5 eV).**

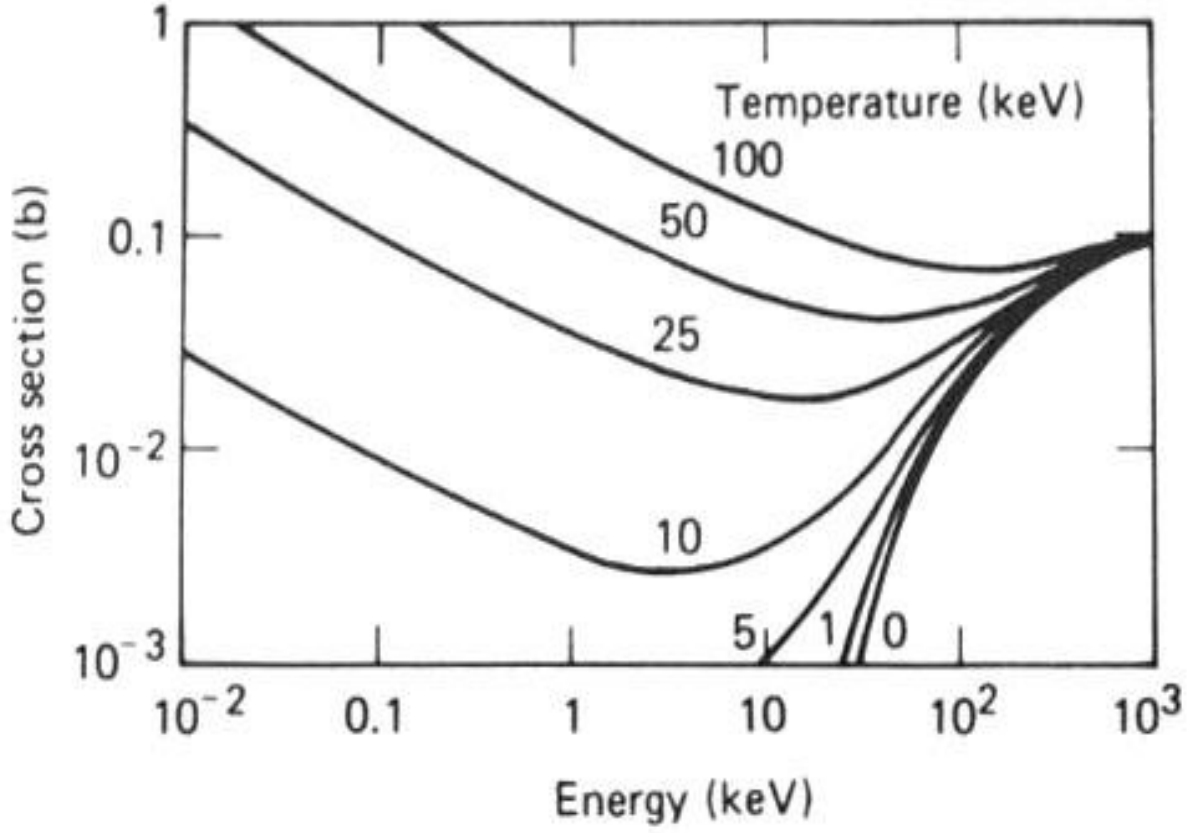




Fusion: (D,D) cross section 0 to 100 keV Temperature

Even at relatively low temperatures C-M threshold reactions will shift slightly downward in the LAB system, as the LAB target speed combines with projectile LAB speed to be above the threshold in the C-M system. For example, at the threshold of an inelastic reaction, the inelastic scattered neutron will in a Maxwellian distribution, not 0 energy. In the resonance region, upscatter can move a neutron from below to above narrow resonances, making it pass through resonances more than once.

Here I present results for very high temperatures, where the (D,D) cross sections with a C-M threshold in the keV range, but with increasing temperature the Lab threshold decreases in energy, and by 10 keV temperature there is no longer a LAB threshold.



One Picture is worth a thousand words

Hopefully the above pictures of ENDF tabulated data clearly illustrates that if you create or use ENDF data graphics should be an integral part of your tool box. Unfortunately, today too many of us assume ENDF data is perfect and no longer "look" at or question this data. ENDF is far from perfect; that is why we have a new versions of ENDF/B every few years. I encourage you not to make the mistake of assuming it is perfect. Instead take a few minutes to look at the data, and if you question anything PLEASE supply feedback – constructive criticism – back to NNDC. Take these few minutes to correct the data now or you will have to live with the current ENDF data for the next few years. Look at the above U238 capture cross section; it would be so easy for you to quickly look at ENDF data like this before you use it; ensure that,

#1: the low energy capture and fission is close to or exactly temperature independent.

#2: the unresolved unshielded average cross sections are smoothly varying; if not this may be a valid physics definition of unresolved, but it is not the correct definition of ENDF unresolved that our processing and application codes expect.

#3: is there the expected discontinuity between the energy dependent resolved and averages in the unresolved.

#4: are there any other (e.g., nuclear model code) cross sections valid at high energy, but here extended downward in energy into the resonance regions that do not show any correlation to the resonances. You should question the validity of this data. Be aware that nuclear model codes cannot accurately predict the location or width of resolved resonances; they can, however, predict the distribution of resonance widths and spacing in the unresolved resonance region.

If the ENDF data you "see" passes these tests you can be confident that the data is valid for use in your applications, i.e., you are not in a "garbage in = garbage out" situation. If not, PLEASE supply feedback – constructive criticism - to NNDC asking that the ENDF data be corrected; this is essential if you are to expect the next version of ENDF to be better than the current version.

Conclusion

Hopefully by now in this report I have said – and repeated – enough details about Doppler broadening to allow the next generation of evaluators, processors, and users of my SIGMA1 method of broadening to understand and carry on from here. If you still have any questions PLEASE free to ask them now – I am 85 years old, so PLEASE ask your questions now, before I disappear from the scene or I have forgotten the answer. If you have any questions or comments concerning ENDF please contact Dave Brown [email: DBrown@bnl.gov]; he is head of NNDC and sole editor of the ENDF bible, ENDF-102 [4].

Please remember that one of the prime reasons for ENDF's great success over the last 60 years has been the close bond between those who produce the data and those that use/test the data, in the form of feedback – constructive criticism. This hopefully will make the next version of ENDF better than the current version. It does indeed take a village, and you the reader of this report are part of that village – so PLEASE HELP.

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[1]"Exact Doppler Broadening of Evaluated Neutron Cross Section," Trans. Amer. Nuc. Soc. 16, p. 320 (1973).

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[7] "**TART 2022**: An Overview of A Coupled Neutron-Photon 3-D, Combinatorial Geometry Time Dependent Monte Carlo Transport Code", Report: LLNL-SM-835527, Code Release: LLNL-CODE-836321, May 2022.

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[14] with Andrej Trkov and Daniel López Aldama, "On the **Self-Shielding** in the **Unresolved Resonance Range**", presented at the 29th International Conference Nuclear Energy for New Europe (NENE 2020), September 7-10, 2020, Portoroz, Slovenia.

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