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EPITHERMAL CAPTURE CROSS SECTION OF $^{235}\text{U}$

A report by the Working Party
on International Evaluation Co-operation
of the NEA Nuclear Science Committee

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NUCLEAR ENERGY AGENCY
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FOREWORD

A Working Party ..... 

The Parties to the ....

The following report was issued by a Subgroup investigating a problem with the early Releases of the ENDF/B-VI evaluated neutron cross sections for $^{235}$U (6.0, 6.1, 6.2). Despite the high quality of the fits to a variety of accurate differential data, thermal benchmarks and other soft-spectrum critical facilities were not well-calculated. It appeared that both thermal-averaged $\eta$ and the capture resonance integral were low, so that low-leakage thermal assemblies calculated low, but with increasing leakage, this trended into a strong overcalculation. It was shown in Release 6.3 that some reasonable adjustments to the Release 2 resonance parameters could remedy the problems, and the Subgroup's objective was to produce a new high-quality fit to the differential data incorporating these findings.

The opinions expressed ...
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SUMMARY

Subgroup 18 was formed to investigate a problem with the early Releases of the ENDF/B-VI neutron cross sections for $^{235}$U (6.0, 6.1, 6.2). Despite high quality fits to accurate differential data, thermal benchmarks were not well-calculated. It appeared that both thermal-averaged $\eta$ and the capture resonance integral were low, so that low-leakage assemblies calculated low, but with increasing leakage, this trended into a strong over-calculation. It was shown in Release 6.3 that a reasonable adjustment to the Release 2 resonance parameters could remedy the problems, and the Subgroup's objective was to produce a new high-quality fit to the differential data incorporating these findings.\(^a\)

This report reviews the evaluation work at Oak Ridge National Laboratory (ORNL), AEERE Harwell and Lockheed Martin Corp.-Schenectady (LMS), which led to ENDF/B-VI Release 5. The important role which benchmark testing in France, the UK, and the US (and elsewhere in the world) played in shaping the final product is mentioned but not in great detail. A large number of published reports give more information, and we apologize to those authors whose work is not explicitly cited.

The current status is as follows: The August 1997 evaluation of Leal-Derrien-Wright-Larson was extensively tested and was adopted for ENDF/B-VI.5 and JEFF-3. It gives good agreement with differential and integral data, and for thermal benchmarks. The calculation of intermediate-energy critical assemblies is improved but more could be done in this important area. The fit to fast benchmarks is unchanged from previous Releases.

A fit to the 0-150 eV region produced by M. C. Moxon at Harwell with the least-squares code REFIT used only differential data and arrived at somewhat different shapes for the thermal-region cross sections and to some extent the resonances also. Coupling this analysis to a set of higher energy cross sections, and to a suitable nu-bar file will permit testing it in practical calculations, a task for the future.

Other topics remaining to be addressed include an improved unresolved-resonance region and a better representation of the energy-dependence of nu-bar. A related issue, which clouds the interpretation of low-enriched $^{235}$U benchmarks, is the question of whether the $^{238}$U thermal and resonance capture cross sections are correct.

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\(^a\) Initially it was thought that only the capture resonance integral adjustment would be addressed, but the group expanded its "charter" to include thermal $\eta$ also. However, the name of the Subgroup was never changed.
$^{235}$U Epithermal Capture

1. Introduction

Subgroup 18 was formed to investigate a problem with the early Releases of the ENDF/B-VI neutron cross sections for $^{235}$U (6.0, 6.1 and 6.2). Despite high quality fits to accurate differential data, documented in Reference 1, thermal benchmarks were not well-calculated. It appeared that both thermal-averaged $\eta$ and the capture resonance integral were low, so that low-leakage assemblies calculated low, but with increasing leakage, this trended into a strong over-calculation. Typical of such calculations are the results in Figure 1, showing a collection of solution-tank eigenvalues calculated with a continuous-energy monte carlo code (Reference A). The introduction of an energy-dependent ("drooping") eta in the sub-thermal region in Releases 1 and 2 improved the calculation of temperature coefficients but did not affect the eigenvalue leakage trend. In Release 6.3 it was shown that some reasonable adjustments to the Release 2 resonance parameters could remedy the problems, and the Subgroup's objective was to produce a new high-quality fit to the differential data incorporating these findings.

Basically, Release 3 (Reference 7) showed that the average radiation width needed to be increased from an average of 35 meV to about 38, and that this could be achieved by giving more weight to the microscopic capture measurements of Reference 8. In addition, it lent strength to the opinion that thermal-averaged eta was being pulled down too much by the CSEWG Standards value of nubar (Reference 5). Initially it was thought that only the resonance integral (epithermal) adjustment would be addressed, but the Subgroup expanded its charter to include thermal $\eta$ also. However, the name of the Subgroup was not changed.

This report reviews the evaluation work at Oak Ridge National Laboratory (ORNL), AERE Harwell and Lockheed Martin Corp.-Schenectady (LMS), which has influenced, or appeared in, ENDF/B-VI through Release 5. The discussion is about the thermal and resolved-resonance regions, and the important role which benchmark testing has played, although the most recent work at Oak Ridge and Harwell concerns the unresolved resonances. A large number of published reports give more detail, and we apologize to those authors whose work is not explicitly cited.

The current status of the $^{235}$U evaluation work is as follows: The August 1997 evaluation of Leal-Derrien-Wright-Larson was extensively tested in France, the UK and the US and achieves the principal objectives of the Subgroup, to agree with both differential and integral data, and to adequately predict the criticality of thermal and intermediate-hardness benchmarks. On this basis, it was adopted for ENDF/B-VI.5 and
for JEFF3. A single Reich-Moore resolved-resonance region, arrived at by Bayesian fitting with the computer code SAMMY, covers the energy range from 10$^{-3}$ eV to 2.25 keV. Agreement is good with differential and integral data, and for thermal benchmarks. The calculation of intermediate-energy assemblies is improved with respect to Release 3. The fit to fast benchmarks is unchanged from previous Releases. Figure 2 illustrates the improvement in eigenvalue leakage trend when Release 6.5 is used.a

An alternative fit by M. C. Moxon at AERE Harwell used the least-squares code REFFIT over the range from 0-150 eV. It relied solely on differential data and arrived at somewhat different shapes for the thermal-region cross sections and to some extent in the resonances also. Figures 3 and 4 compare the fission and capture cross sections from this evaluation with the L-D-L-W values in the 0-1 eV region. Differences in the fission are visible, and are quite pronounced in the capture. In order to test Moxon's work in practical calculations, it will be necessary to couple it to a set of higher energy cross sections, and to a suitable nu-bar file, a task for the future.

Some important topics remain to be addressed, primarily an improved treatment of the unresolved-resonance region and an improved representation of the energy-dependence of nu-bar. A related issue, which clouds the interpretation of low-enriched $^{235}$U benchmarks, is the question of whether the $^{238}$U thermal and resonance capture cross sections are correct. These and some other topics for future consideration are discussed in the Appendices.

2. Review of $^{235}$U neutron cross section evaluation work

2.1 ENDF/B-VI.0

The original Releaseb of ENDF/B-VI.0 $^{235}$U in 1990 was a collaboration among the Oak Ridge, Los Alamos, and Argonne National Laboratories, the last two providing the high-energy cross sections, and ORNL the resonance analysis. The latter culminated in an extensive Reich-Moore multilevel fit to the resolved-resonance region 0-2250 eV.1

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*aFurther improvement results from the use of Release 6.5 hydrogen capture, down from 332.6 mb in Releases 0-4, to 332.0, but not included in the Figure 2 values.

*bSuccessive versions of ENDF/B-VI materials are designated as Mods. $^{235}$U has undergone modification in every Release of ENDF/B-VI, so the Mod number, which started as 1 in Release 0, is one greater than the Release number. We use the latter, as more familiar to most users. (The number of Releases, and the fact that different ones may contain quite different cross sections, makes it important for users and authors of technical articles to insure adequate identification of which ENDF/B-VI materials they used. The term ENDF/B-VI by itself is not unique.)
The work was carried out with the powerful resonance-fitting code SAMMY,\textsuperscript{2} which uses Bayes' method for the fitting procedure, making it possible to deal sequentially, yet consistently, with the many large data sets requiring analysis. The evaluation techniques were a major advance over the earlier single-level treatments in ENDF/B-I through V, the latter of which ended the resolved region at 82 eV and treated the thermal region (0-1 eV) as tabulated data in File 3. The ENDF/B-VI evaluators recognized that the experimentally-observed structure in the cross sections above 100 or 150 eV was largely due to clumps of resonances, but it was their opinion that fitting it as if it were resolved "pseudo-resonances" would preserve the structure and permit users to derive more accurate estimates for self-shielded multigroup cross sections than could be inferred from a traditional treatment in terms of average unresolved resonance parameters. This important question has never been settled, and remains one of the tasks for future investigation.

In the Cross Section Evaluation Working Group (CSEWG) review procedure, which was quite extensive, involving special meetings at Oak Ridge, the Thermal Benchmark Testing Subcommittee, under the chairmanship of J. R. Hardy and (later) M. L. Williams, observed that there were two "differential-integral" discrepancies which affected the evaluation:\textsuperscript{3}

1. The 2200 m/s values for capture and fission, and their associated Westcott g-factors, produced a Maxwellian-averaged \( \eta \) (\( \nu \)-fission/absorption) which was lower than the value inferred from eigenvalue calculations of thermal reactors. Quantitatively, the effect was measured by the parameter \( K_1 = \nu \sigma_{\text{fission}} - \sigma_{\text{absorption}} \) (in which the cross sections are the Westcott Maxwellian-averages, g-factor times 2200 m/s value). The integral value derived from an analysis of the Gwin-Magnuson aqueous assemblies was 722.7±3.9 whereas the evaluation gave about 719\textsuperscript{c}. The 2200 m/s values were the then-recommended thermal constants that resulted from an extensive round of least-squares fitting to pointwise and reactor-averaged thermal data, following a tradition started many years earlier by G. H. Westcott. The CSEWG discussions of the least-squares results were spirited. Within the CSEWG Task Force on Thermal Constants, led by B. R. Leonard and J. R. Stehn, some believed that least-squares was the best one could do, while others believed that the results were too sensitive to the choice of input uncertainties, and that the output uncertainties were unrealistically low. It was noted that the main input data at the low-\( K_1 \) end were the Chalk River reactor-average-alpha measurements, which were high and carried low uncertainties, and some low nubar data.

\textsuperscript{c} The calculations leading to the value 722.7 do not appear to have been published in the open literature. The methods used are described in internal CSEWG correspondence and in unpublished laboratory memoranda. Current experience with thermal benchmarks supports the value.
A complete discussion of the relevant data can be found in Reference 4, where an exhaustive least-squares fit to the thermal constants resulted in $K_1 = 712.6$. That low value epitomized the integral-differential conflict for $^{235}$U.

That disagreement in philosophy is still with us, and as recent experience has shown, a straightforward fit to the thermal "differential" data still yields a $K_1$ which is below the integral value.\(^5\) The result of the low $K_1$ was that eigenvalues (multiplication constants) for well-thermalized assemblies calculated around 0.5% low using Release 0.

2. The resonance integral for radiative-capture was some 10 barns below the integral value of about 142 barns. Correspondingly, its ratio to the fission integral, (epithermal alpha) was 6-7% below the integral value of 0.51. A consequence of this fact, and of the low $K_1$, was that Release 0 calculated low multiplication constants for very-thermal, large, low-leakage assemblies, but the calculated values rose sharply with increasing leakage, as shown in Figure 1. As the leakage increased, and the spectrum hardened, the low alpha caused the calculated eigenvalues to increase. Nevertheless, the evaluation was accepted for ENDF/B-VI.0. One reason was a matter of principle among many of the CSEWG members that ENDF should represent a pure view of the microscopic measurements, and not allow itself to be influenced by integral considerations, which (then, and still today) can manifest themselves in ad hoc adjustments to cross sections, without a clear physical basis. M. L. Williams has also pointed out, in Reference E, that benchmark (Phase II) testing was hampered by a lack of suitable processing codes and of adequate funding.

Another consideration, as valid today as it was then, is whether the integral data are accurate. Perhaps the thermal benchmarks are afflicted with some unknown error, and that in fact the low $K_1$ resulting from a least-squares fit to the microscopic measurements is correct. It would be undesirable to change the evaluation in order to fit incorrect benchmarks.

It is impossible to answer this criticism. However, one cannot simply ignore the integral measurements, so in the recent evaluation activities at ORNL and LMS a more pragmatic attitude has been adopted. Essentially, the argument is that all the experiments are "wrong," if by "right" one means they give the "true" value. The microscopic measurements can only define an envelope of credibility, and it is possible to stay within that envelope and still match the integral data. In particular, "pure" least-squares fits to the microscopic data are to be preferred only in the absence of other indications. The weakest links in the microscopic measurements appear to be the normalization of capture measurements and the specification of the true resolution in measurements of the ratio alpha. In the fitting process, one is severely limited in the extent to which a "true" radiation width can be extracted from the Doppler and resolution-broadened data. In the
most recent contributions from Leal, et al, and from M. C. Moxon (Sections 2.10 and 2.11), the radiation width is constrained to be either exactly equal to, or very close to, an average value of about 38 meV. Insofar as that value is itself determined by the differential data, these procedures are in the direction of reducing reliance on integral quantities.

Finally, present evaluation methods assume a constant value of nubar in the thermal region, and that value is not simultaneously fit. It seems reasonable that adding a fit to an energy-dependent nubar would allow better fits to thermal benchmark eigenvalues without as large an effect on the cross sections.

In the most recent evaluation from ORNL (August 1997), which has been adopted for ENDF/B-VI Release 5, integral data have been incorporated into the basic fitting process, by adding to SAMMY the ability to fit integral values, in particular, resonance integrals and K1. This provides a mathematical bridge between the two worlds, but puts an added burden on the evaluator to insure the results are physically reasonable. The procedure provides better representation of the integral data while maintaining the excellent fit to the differential data (see Section 2.10)

2.2. ENDF/B-VI.1

Release 1 (1991) introduced an energy-dependence in sub-thermal eta, so-called "drooping eta." The possibility of such an energy-dependence had been hypothesized by Santamarina, et al., and later confirmed by measurements at Geel, Harwell and ORNL. This modification removed most, but not all, of the discrepancy between measured and calculated temperature coefficients which had stimulated the original investigation. Since no other modifications were introduced, Release 1 continued to test poorly on thermal benchmarks. Like Release 6.0 before it, the resolved-resonance region was split into eleven sub-regions, covering the energy range 0.00001 - 2250 eV.

2.3. ENDF/B-VI.2

Release 2 (1993) did not change the cross sections.

2.4. ENDF/B-VI.3

Release 3 (1995) was an adjustment to Release 2, carried out at LMS by C. R. Lubitz. This adjustment increased the epithermal capture to agree, on average, with the measured differential capture cross sections of Perez and deSaussure, and also increased K1 to improve the calculation of the very-thermal assemblies; details of the adjustment process are provided in the report. Because it was an adjustment to average cross sections over energy bins, the improvements came at the expense of decreasing the agreement with the detailed differential measurements.
As expected, Release 3 did quite well on the thermal benchmarks, raising eigenvalues for the very thermal cores, and greatly reducing the trend with leakage. Since the cross sections above 900 eV are identical to Release 2, its calculated fast benchmark eigenvalues are also identical. A. Jonsson, at the 1995 CSEWG meeting, reported improvements in reactivity enrichment dependence, and other groups reported similar positive findings. However, Release 3 did not do well on intermediate-spectrum cores, calculating 1-2% high on the HISS(HUG) and the two UH3 benchmarks which RQ Wright had added to the set of benchmarks being used to test $^{235}$U. One can speculate that the same “low-alpha syndrome” which affected Release 2 below 900 eV extends up much higher in energy.

The adjustment process, which was done using bin-averaged cross sections, maintained the discontinuities in the unbroadened cross sections at the resonance-subregion boundaries. Although smoothed out by subsequent Doppler-broadening in the processor code NJOY, they remained an unattractive feature. Release 3 also had a formatting error in that the increased value of thermal nubar was put into the total-nubar file, but not into the prompt-nubar file. That meant that processing codes like MCNP which reconstituted the total from prompt + delayed got slightly lower thermal eigenvalues than they should have (nubar = 2.4320 instead of 2.4338, or 74 pcm).

2.5. ENDF/B-VI.4

ENDF/B-VI Release 4 (1996) is the same as 3, but corrected the prompt nubar file.

2.6. Leal-Derrien-Wright January 1996

In January of 1996, Oak Ridge (L. C. Leal, H. Derrien and R. Q. Wright) completed a preliminary re-evaluation from 0 to 2.25 keV, which put all the resonances into one region, thus eliminating the need for carefully tailoring “external” resonances in each of the previous eleven regions. The evaluation covered most available differential data (two sets of fission plus capture data, one fission plus absorption, six fission alone, two transmission). The new work matched the higher epithermal alpha and K1 of Release 3, and in addition provided excellent detailed fits to the differential data. It did well on the thermal benchmarks and in addition produced better (lower) eigenvalues for the three intermediate-spectrum HISS(HUG) and UH3 cores.

2.7. Leal-Derrien-Wright-Moxon March 1997

However, there was room for improvement: M. C. Moxon (and others) observed that the radiation widths fluctuated more than was expected theoretically. He also questioned whether the target backings had been adequately accounted for in the
experimental and evaluation phases of the work, and whether the free-gas model was adequate for Doppler-broadening the low-energy resonances⁴.

To help resolve these questions, Moxon spent two months at ORNL in late 1996. He and N. M. Larson worked to reconcile numerical and procedural differences between Moxon's code REFIT¹² and SAMMY. All numerical constants were made consistent. Detailed comparisons among SAMMY,² REFIT,¹² NJOY,¹⁰ and other codes led to a more accurate treatment of the low-energy free-gas model for Doppler-broadening in REFIT.¹³ Nevertheless, Moxon's Doppler question still remains; crystalline-binding models provide a better description of low-energy Doppler broadening than a free-gas, but the effect is probably more important for ²³⁸U than for ²³⁵U, for which more important effects are still not adequately understood. Since crystalline-broadening is not yet available in ENDF-processing codes, it was decided to continue the work with the free-gas model.

Other differences between SAMMY and REFIT, besides the use or non-use of Bayesean methods, remain. Examples are the way in which the neutron-burst moderation is calculated; the way the resolution function is synthesized from its components; and the multiple-scattering correction to capture and fission yields (included in both codes but implemented differently). The practical impact of such differences has not been assessed, and there is currently no support for further harmonization of the two codes. It should be emphasized however, that the existence of two such sophisticated analysis tools, and the expertise which their authors and users have brought to bear on the ²³⁵U cross sections, have resulted in higher-quality fits than was possible as recently as five years ago.

During Moxon's stay at Oak Ridge, Leal, Derrien and Moxon, together with J. A. Harvey and R. Spencer of ORNL, and M. Moore of LANL, were able to answer most questions regarding the ORNL experimental data-reduction procedures. The resulting data set received limited testing by Dean et al.,¹⁴ plus unpublished work by Wright, Kahler and Weinman. The consensus was that the benchmark behavior was reasonable, but more should be done.

2.8. Leal-Derrien-Wright May 1997

Subsequently, Leal, Derrien, and Wright produced an interim set for discussion at the May 1997 Cadarache meeting of the WPEC. The generation of this set utilized a new capability in SAMMY, allowing the inclusion of integral data (resonance integrals and

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⁴ The fluctuations were reduced in subsequent fits by constraining SAMMY's search region. ORNL confirmed that the backings had been properly treated, and practical considerations made it desirable to ignore crystalline binding effects for the present.
K1) within the fitting procedure, thus putting this phase of the work on a more objective basis.

2.9. Moxon May 1997

Independently, Moxon produced a fit to the 0-100 eV region that differed from previous $^{235}$U evaluations in having a rather low capture g-factor, about 0.95 instead of the traditional 0.99. This may have been the result of removing the original normalization and background from the 1966 deSaussure capture and fission data\textsuperscript{15} and re-fitting it with REFIT. Like the May 1997 ORNL fit, this was an interim version, for discussion at the Cadarache meeting. The only action taken there was to recommend that an attempt to reach a consensus would be made before the October 1997 CSEWG meeting. That turned out not to be possible, and the two evaluation efforts are still separate.

A relatively low Maxwellian-averaged fission in Moxon's data set outweighed the low capture g-factor, and implied a low K1 unless it could be coupled with a nubar much higher than the ENDF/B-VI Standards value. Such a higher nubar (2.4374) exists in the measurements of Gwin, et al.\textsuperscript{16}, which has already been adopted by both the Joint European File (JEF) and the Japanese Evaluated Nuclear Data Library (JENDL). At LMS, Lubitz tested a "tri-partite" data set, obtained by inserting Moxon's fit from 0-10 eV into the January 1996 ORNL evaluation, and replacing the nubar file with the JEF values. Benchmark testing showed that such a hybrid set performed satisfactorily on thermal benchmarks, but did poorly on the harder-spectrum cases. It appeared that the higher Gwin nubar "worked" for the soft-spectrum cases, but was too high for the others. These conclusions need to be more closely examined. An interesting question is whether the different capture shape which produces the low g-factor in Moxon's work will affect temperature coefficients.

2.10. Leal-Derrien-Wright-Larson August 1997

After the WPEC meeting at Cadarache, Leal and Derrien continued to refine their fits, and in August, 1997 a new data set was made available for testing. It incorporated the integral-quantity fitting capabilities of SAMMY to deal with the earlier problems of low K1 and epithermal alpha. Most noticeably, thermal nubar was increased from the Release 3 value (2.4338) to 2.4367 over the range from 0 to 1 eV. This value was arrived at by treating thermal nubar as a search parameter in the SAMMY runs, while using the benchmark value of K1 as a quantity to be fitted. The value 2.4367 is close to a smooth average through the fluctuating Gwin data points in this interval, and is also (fortuitously) exactly the ENDF/B-V value. By cutting off the increase at 2 eV, the fit avoids the deleterious effect of a higher nubar on the harder-spectrum cores. The radiation widths in the new L-D-W-L data set have an average value over 0-100 eV of
about 40 meV, with a standard deviation of 10%. It seems reasonable to expect that on average the capture will be the same from such a narrow distribution as from a constant radiation width, making this an acceptable degree of fluctuation.

At the October 1997 CSEWG meeting, A. C. Kahler and J. P. Weinman presented benchmark results with this new data set, for about 25 benchmarks including ORNL spheres and cylinders, ORNL L-series, Rocky Flats, HISS(HUG), and two UH3 intermediate-spectrum cases. The best results were obtained using a reduced hydrogen capture cross section, 332.0 mb instead of 332.6, and a slightly-modified version of ENDF/B-VI oxygen, which had more forward scattering. The effect of the hydrogen was to raise the low-leakage end of the thermal benchmark “trend line” about 100 pcm, while the additional oxygen leakage lowered the high-leakage end about the same amount. Together they produced a flat trend line with an average eigenvalue very close to unity. The intermediate-spectrum cases are close together at about 1% high. The thermal cases are therefore about the same as Release 3, while the 3 harder cores are better, although not quite as close to unity as in the January 1996 evaluation of Leal-Derrien-Wright. In view of its good benchmark performance, it was accepted for inclusion in ENDF/B-VI Release 5 (as was the new hydrogen capture.) A decision on the oxygen is awaiting completion of a new evaluation at Los Alamos National Laboratory by G. Hale.

In December of 1997, two papers were presented at a meeting of the JEF Working Group on Data Evaluation and Benchmark Testing. Both showed significant improvements using L-D-W-L over the JEF2.2 data set, which is similar to ENDF/B-VI Release 2. The studies covered a wide range of quantities, among them buckling measurements, k-infinities, temperature-dependent Westcott g-factors, and spent-fuel analyses. In each area the L-D-W-L set improved the agreement between calculation and experiment. Of particular interest were the spent-fuel results, since they test the cross sections in a way that is relatively independent of any remaining problems with nubar. As a result of these favorable findings, the new data were adopted for JEFF3.

Complete details of the L-D-W-L evaluation were given in an ORNL report, and a slightly abbreviated version in the open literature. Details of the inclusion of integral quantities into the analysis were also published as an ORNL report and in the open literature.

2.11. Moxon September 1997

Moxon has released a version of his latest work to the Nuclear Energy Agency Data Bank at Paris. It extends his earlier work to higher energies, and achieves satisfactory fits to the differential data using a single value of the radiation width, close to the 38.2 mV he recommended in Reference 25. As of this date, it has not been reviewed or benchmark tested, since that will require it to be coupled with a nubar file and higher
energy cross sections. Moxon's work represents a "pure" fit to the microscopic data, so that if it is to be useful in integral calculations, it will probably require a new treatment of nubar. That is also a topic for further investigation, as is the significance of the unusual Westcott g-factor for capture, noted above in connection with his May 1997 work. The work utilizes a J-dependent scattering radius, and the ENDF formats and processing codes should be expanded to treat this as-yet not "allowed" feature.

2.12. The Role of Integral Testing

The degree to which successive Releases of ENDF/B-VI agreed or disagreed with various integral benchmarks has from the start been an essential element in shaping its development. With the evolution of Release 3 and subsequent refinements, that aspect of the evaluation process became more integrated into the data-fitting process. At Oak Ridge, R. Q. Wright routinely checked successive iterations of the differential-data fitting and/or adjustment process, and provided feedback on their integral adequacy. At Bettis Atomic Power Laboratory and at LMS, A. C. Kahler and J. P. Weinman continuously monitored the progress with highly-accurate point-energy Monte Carlo calculations. The major Releases were checked by the CSEWG Thermal and Fast Reactor Testing Subcommittees under M. L. Williams (LSU) and R. D. McKnight (ANL). R. D. Mosteller at Los Alamos National Laboratory used both CSEWG benchmarks and the newer collection embodied in the International Criticality Safety Benchmark Evaluation Project under J. Blair Briggs (INEL) to assess both ENDF and other data sets. Large-scale calculation of both published and proprietary benchmarks were carried out by the UK, France, Japan, and elsewhere.\textsuperscript{14,18,19,20-28} The reader is referred to the minutes of the annual CSEWG meetings at Brookhaven, to the transactions of the annual and topical meetings of the American Nuclear Society, and to the proceedings of the International Conferences on Nuclear Data for Science and Technology, for Basic and Applied Science, for Reactor Safety, and related meetings.

Because of the many different methods used to measure the benchmarks and to calculate them, and because many of them are proprietary, it is difficult to incorporate the results directly into the evaluation process. Instead they provide broad-brush indications of where problems exist, and can focus the evaluators' attention on the appropriate differential data.

3. Current Status of $^{235}\text{U}$ Evaluation

The current ENDF/B-VI evaluation$^{20,21}$ (Release 5) reaches some important goals:

1. The problems concerning the capture cross section in the earliest Releases are understood:
a. An average capture width\(^\text{29}\) of 38.03±1.70 meV in the range from 0 to 50 eV was obtained from the SAMMY\(^\text{2}\) analysis of a large set of experimental differential data, based on well-resolved time-of-flight experiments. This agrees with the value (38.2±??) originally obtained by M. C. Moxon from an analysis of selected resonances in 0-20 eV (Reference 25), and with the value (38.2) obtained independently in Release 3 (0-100 eV) by adjusting the Release-2 capture cross section upwards to match the bin-averaged capture of Reference 8.

b. The average capture width increased to 39.4±2.0 (+3.6%) when integral data were added to the experimental data base.\(^\text{29}\) This (final) value agrees with the above to within the uncertainty.

c. The capture resonance integral obtained from these parameters is 140.9 b, giving an alpha value of 0.509, consistent with integral measurements.

d. The capture widths show fluctuations on the order of 10%. Such fluctuations are considered to be acceptable in order to provide the best possible fit to the differential data. Moxon has arrived at an alternative fit using a fixed value of the radiation width, achieving comparable \(\chi^2\) (goodness-of-fit) values, but at present there is no evidence indicating a technological difference between the two approaches.

2. Combining the resonance parameters into one region has eliminated the problem of discontinuities between the eleven sub-regions in previous ENDF/B-VI releases. This simplifies the representation of the distant level contribution.

3. The ORNL evaluation\(^\text{10}\) reproduces below 0.1 eV the shape of eta predicted by Santamarina.\(^6\) The Gwin 1990 eta data (Reference C) are well reproduced in the energy range below 1 eV. The only problem is from the Wartena data (Reference B) in the high energy wing of the 0.3 eV resonance where the data are questionable.

4. Good agreement is obtained in benchmark results for highly-enriched thermal assemblies and improved results for intermediate spectrum cases. Studies continue to show poorer agreement in low-enrichment cores, but that effect cannot be reliably disentangled from the \(^{238}\)U cross section questions.

5. The necessity to treat nubar without a theoretical shape continues to be an undesirable aspect of the evaluation process. JEF and JENDL have adopted "raw" discontinuous experimental data, and L-D-L-W used it to "fit" the parameter K1. An improvement is needed in this area (see below).
4. Topics for Future Investigation

1. Resonances above 100 to 150 eV are only partially resolved, but are parameterized in ENDF/B-VI as if they were actual resonances. The effect of these pseudo-resonances on the accuracy of the calculated self-shielding effects should be examined, and compared with a conventional treatment in terms of average parameters.

2. The unresolved resonance region should be re-evaluated, using Reich-Moore and taking into account the very accurate total cross section obtained from Harvey's transmission data\textsuperscript{31}; this could modify the fission and/or the capture cross sections by a few percent. A preliminary multilevel fit has been carried out by Moxon and shows a significant increase in $\alpha$ relative to an SLBW treatment (Reference D). Similar work is in progress at ORNL.

3. The ENDF/B-VI fission standard should be reconsidered.\textsuperscript{32} If this standard is retained with its claimed accuracy, then the inconsistency between it and the ENDF/B-VI.5 evaluation remains to be resolved, and the problems concerning the capture cross section could reappear. The problem will also show up in the unresolved resonance region. The current standard is based on the alpha measurements of Corvi\textsuperscript{33} and of Muradyan\textsuperscript{34}; the important data of Beer\textsuperscript{35} obtained at Karlsruhe with a very high resolution were not considered. These data, in excellent agreement with deSaussure\textsuperscript{36} data, are 6 to 7% higher than the Corvi data. Taking for alpha an average value of Corvi, Beer and de Saussure will give fission cross sections 2-3% smaller than the standard values, if the total cross section is kept at the accurate Harvey value.

4. Possible variation of nubar in the resonances was not considered in the ORNL (Release 5) evaluation. Both theory and experiment show that nubar varies from resonance to resonance, yet that variation is universally ignored in the cross section evaluation process.\textsuperscript{16,37-41} The current good fits to capture, fission and total cross sections suggest that these are now "well-known" and are incompatible with integral reactivity measurements unless coupled to a much higher nubar than has been used in earlier Releases of ENDF/B-VI. Introducing a sound theory-based description of the energy-dependence of nubar could have a beneficial effect on many calculations, since it would open up an important new degree of freedom. Any correlation between nubar and alpha could affect both the thermal and intermediate-spectrum calculations. Other areas would be discrepancies between $\alpha$- and $\eta$-measurements, and calculated temperature coefficients.

5. Crystalline Doppler broadening is currently under intense scrutiny for $^{238}$U, but it has not been shown to be of comparable importance for $^{235}$U. M. C. Moxon has used an
Einstein model in REFIT to achieve better fits to the wings of the low-energy resonances in $^{235}\text{U}$, but a test of that refinement in reactor calculations has not been carried out.

6. There does not appear to be any calculation that would test the degree of fluctuation in the radiation widths. As noted above, using a constant width, or a narrow distribution, appear to be technologically indistinguishable.

7. More intermediate-energy benchmarks are needed to test the evaluation, and in general more effort needs to go into understanding discrepant results from different organizations. First priority should go to highly-enriched, homogeneous assemblies.

8. The question of over-absorption in $^{238}\text{U}$ continues to cloud benchmark results for low-enriched $^{235}\text{U}$. Modern computational techniques, most importantly accurate point-energy Monte Carlo calculations, could settle the issue of whether the basic data are responsible, or whether the problem is in the reduction to multigroup cross sections and related calculational approximations.

5. Conclusions

An extensive effort has gone into the evaluation and testing of the $^{235}\text{U}$ resonance region since the start of ENDF/B-VI in 1990. In Release 5 we have arrived at a credible data set that fits a variety of both differential and integral data. Some questions remain, such as the extension of better methods to the unresolved region, incorporating a theory and experiment-based variation of nubar, objectively deciding whether in fact the pseudo-resonances are superior to an accurate, conventional fit using average parameters based on channel fission theory, and clarifying the role of $^{238}\text{U}$ cross sections in LEU benchmarks.
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Figure 1. Eigenvalues of homogeneous critical assemblies vs. leakage, (Oak Ridge and Rocky Flats). Calculated by continuous-energy Monte Carlo, using ENDF/B-VI Release 0 cross sections.
Figure 2. Eigenvalues of homogeneous critical assemblies vs. leakage. (Oak Ridge and Rocky Flats). Calculated by continuous-energy Monte Carlo, using ENDF/B-VI Release 5 cross sections.
Figure 3. A comparison of the fission cross section below 1 eV from ENDF/B-VI.5 and Moxon.
Figure 4. A comparison of the capture cross section below 1 eV from ENDF/B-VI.5 and Moxon.