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EPITHERMAL CAPTURE CROSS-SECTION OF ^{235}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
ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

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FOREWORD

A Working Party on International Evaluation Co-operation was established under the sponsorship of the OECD/NEA Nuclear Science Committee (NSC) to promote the exchange of information on nuclear data evaluations, validation and related topics. Its aim is also to provide a framework for co-operative activities between members of the major nuclear data evaluation projects. This includes the possible exchange of scientists in order to encourage co-operation. Requirements for experimental data resulting from this activity are compiled. The Working Party determines common criteria for evaluated nuclear data files with a view to assessing and improving the quality and completeness of evaluated data.

The parties to the project are: ENDF (United States), JEF/EFF (NEA Data Bank Member countries) and JENDL (Japan). Co-operation with evaluation projects of non-OECD countries, specifically the Russian BROND and Chinese CENDL projects, are organised through the Nuclear Data Section of the International Atomic Energy Agency (IAEA).

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 and 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 η (nu-fission/ absorption) and the capture resonance integral were low, so that low-leakage thermal assemblies calculated low, but with increasing leakage, the consequent hardening of the spectrum created a trend of strong over-calculation. It was shown in Release 6.3 that a reasonable adjustment to the Release 6.2 resonance parameters could remedy both difficulties, and the objective of the Subgroup was to produce a new high-quality fit to the differential data incorporating these findings.

The opinions expressed in this report are those of the authors only and do not necessarily represent the position of any Member country or international organisation. This report is published on the responsibility of the Secretary-General of the OECD.

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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 and 6.2). Despite high quality fits to accurate differential data, thermal benchmarks were not well calculated. It appeared that both thermal-averaged η (nu-fission/absorption) and the capture resonance integral were low, so that the multiplication constants ("eigenvalues") of low-leakage assemblies calculated low, but with increasing leakage, the consequent hardening of the spectrum created a trend of strong over-calculation. It was shown in Release 6.3 that a reasonable adjustment to the Release 6.2 resonance parameters could remedy both difficulties, 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), Atomic Energy Research Establishment (AERE) Harwell, and Lockheed Martin Corp. (LMC) which led to ENDF/B-VI Release 6.5. 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 apologise to those authors whose work is not explicitly cited.

The current status is as follows: The Leal-Derrien-Wright-Larson evaluation (August 1997) using the Bayesean-fit code SAMMY, was extensively tested and was adopted for ENDF/B-VI Release 6.5 and JEFF3. It gives good agreement with differential and integral data, and for thermal benchmarks. The calculation of intermediate-energy critical assemblies is improved relative to most earlier versions, 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

[a] Initially it was thought that only the capture resonance integral adjustment would be addressed, but the group expanded its "charter" to include thermal η also. However, the name of the subgroup was never changed.

resonances also. Coupling this analysis to a set of higher energy cross-sections, and to a suitable nubar (average number of neutrons per fission) 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 nubar. 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.

EPITHERMAL CAPTURE CROSS-SECTION OF ^{235}U

1. Introduction

As noted in the summary, Subgroup 18 was formed to investigate a problem with Releases 6.0, 6.1 and 6.2 of the ENDF/B-VI neutron cross-sections for ^{235}U. The fits to differential data documented in References [1] and [2] appeared to produce low values for both thermal-averaged η and the capture resonance integral, so that the multiplication constants ("eigenvalues") of low-leakage assemblies calculated low, but with increasing leakage, trended to strong over-calculation. Typical of such calculations are the results in Figure 1, showing a collection of solution-tank[b] eigenvalues calculated with a continuous-energy Monte Carlo code [3]. The introduction of an energy-dependent ("drooping") η in the sub-thermal region in Releases 6.1 and 6.2 improved the calculation of temperature coefficients but did not help the eigenvalues. In Release 6.3 [4] it was shown that a reasonable adjustment to the Release 6.2 resonance parameters could remedy both problems, and the Subgroup's objective was to produce a new fit to the differential data incorporating these findings.

Basically, Release 6.3 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 in Ref. [5]. In addition, it lent strength to the opinion that thermal-averaged η was being pulled down too much by the Cross-Section Evaluation Working Group (CSEWG) standards value of nubar [6].

This report reviews the evaluation work at ORNL, AERE Harwell and LMC which has influenced ENDF/B-VI through Release 6.5. The discussion concerns 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

[b] The Rocky Flats assemblies are numbered according to the International Handbook of Evaluated Criticality Safety Benchmark Experiments [35] and not the CSEWG benchmark numbering system.

reports give more detail, and we apologise to those authors whose work is not explicitly cited.

The current status of the ^{235}U evaluation work is as follows: The evaluation of Leal-Derrien-Wright-Larson (August 1997) was extensively tested in France, the UK and the US. It achieves the principal objectives of the subgroup, specifically, 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 Release 6.5 and for JEFF3. A single Reich-Moore resolved-resonance region, arrived at by Bayesean fitting with the computer code SAMMY [7], covers the energy range from 10^{-5} 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 6.3. The fit to fast benchmarks is unchanged from previous Releases. Figure 2 [8] illustrates the improvement in eigenvalue leakage trend when Release 6.5 is used[c].

An alternative fit by M.C. Moxon at AERE Harwell used the least-squares code REFIT 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 ENDF/B-VI Release 6.5 values used by Leal-Derrien-Wright-Larson (see Section 2.10) in the region below 1 eV. Differences in the fission are visible, and are quite pronounced in the capture. Numerical values for the thermal cross-sections and g-factors for this and other evaluations are given in the table at the end of this report.

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 nubar 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 nubar. 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.

[c] Further improvement results from the use of Release 6.5 hydrogen capture, down from 332.6 mb in Releases 6.0-6.4, to 332.0, but not included in the Figure 2 values.

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

2.1 ENDF/B-VI Release 6.0

The original release[d] of ENDF/B-VI Release 6.0 ^{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 [1,2]. The work was carried out with the powerful resonance-fitting code SAMMY, which uses Bayes' method for the fitting procedure and makes 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 recognised that the experimentally observed structure in the cross-sections above 100 or 150 eV was largely due to clumps of resonances. However, it was their opinion that fitting it as if it were the result of individual resolved "pseudo-resonances" would preserve the structure and lead to more accurate self-shielded multi-group cross-sections than could be obtained 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 CSEWG review procedure, which involved 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 [9]:

1. The 2 200 m/s values for capture and fission, and their associated Westcott g-factors, produced a Maxwellian-averaged η which was lower than the value inferred from eigenvalue calculations of thermal reactors. Quantitatively, the effect was measured by the parameter $K1 = \nu\sigma_{fission}-\sigma_{absorption}$ (in which the cross-sections are the Westcott Maxwellian-averages, g-factor times 2 200 m/s value). The integral value derived by Hardy from an analysis of the Gwin-Magnuson aqueous assemblies was 722.7±3.9, whereas the ENDF file gave about

[d] Successive 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 6.0, 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.)

719[e]. The 2 200 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. On the other hand, some 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-K1 end were the Chalk River reactor-average-alpha measurements, which were high and carried low uncertainties, and some low nubar data. A complete discussion of the relevant data can be found in [10], where an exhaustive least-squares fit to the thermal constants resulted in K1 = 712.6. That low value epitomised 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 K1 which is below the integral value [6]. The result of the low K1 was that eigenvalues (multiplication constants) for well-thermalised assemblies calculated around 0.5% low using Release 6.0.

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 K1, was that Release 6.0 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 Release 6.0. 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 that benchmark (Phase II) testing was hampered by a lack of suitable processing codes and adequate funding [11].

[e] The calculations leading to the value 722.7 were not 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.

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 K1 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 LMC 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 normalisation 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 Moxon (Sections 2.10 and 2.11), the radiation width is constrained to be either very close to, or exactly equal 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 plausible that adding a fit to an energy-dependent nubar would allow improved 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 6.5, 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 ensure 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 Release 6.1

Release 6.1 (1991) introduced an energy-dependence in sub-thermal η, so-called "drooping η". The possibility of such an energy-dependence had been hypothesised by Santamarina, *et al*. [12], and later confirmed by measurements

at Geel, Harwell and ORNL [13]. This episode was an early example of the closer international co-operation on evaluation activities fostered by the Organisation for Economic Co-operation and Development's Nuclear Energy Agency (OECD/NEA) which has proven so fruitful.

This modification removed most, but not all, of the discrepancy between measured and calculated temperature coefficients which had stimulated the original investigation. However, since no other modifications were introduced, Release 6.1 continued to test poorly on thermal benchmark eigenvalues. As with 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 Release 6.2

Release 6.2 (1993) did not change the cross-sections.

2.4 ENDF/B-VI Release 6.3

Release 6.3 [4] was an adjustment to Release 6.2, carried out at LMC by C. R. Lubitz, in close collaboration with J.A. Harvey, A.C. Kahler, N.M. Larson, L.C. Leal, M.C. Moxon, J.P. Weinman, L.W. Weston and R.Q. Wright. This adjustment increased the epithermal capture to agree, on average, with the measured differential capture cross-sections of Perez and de Saussure [5] and it 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 measured over energy bins, the improvements came at the expense of decreasing the agreement with the detailed differential measurements.

As expected, Release 6.3 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 6.2, its calculated fast benchmark eigenvalues are also identical. A. Jonsson reported improvements in reactivity enrichment dependence [14] at the 1995 CSEWG meeting, with other groups reporting similar positive findings. Release 6.3 did not do well on intermediate-spectrum cores, however, calculating 1-2% high on the HISS (HUG) and the two UH3 benchmarks which RQ Wright had added to the set being used to test ^{235}U. It is possible that the "low-alpha syndrome" which affected Release 6.2 below 900 eV extends up higher in energy, but the results are also sensitive to possible errors in nubar.

The adjustment process, which was done using bin-averaged cross-sections, maintained the discontinuities in the unbroadened cross-sections at the resonance sub-region boundaries. Although smoothed out by subsequent Doppler broadening in the processor code NJOY [15,16], they remained an unattractive feature. Release 6.3 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 [17] 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 Release 6.4

ENDF/B-VI Release 6.4 (1996) is the same as Release 6.3, but corrected the prompt nubar file.

2.6 Leal-Derrien-Wright – January 1996

In 1994, H. Derrien was sponsored by CEA Cadarache, Électricité de France and NEA to work at ORNL with O. Bouland on ^{240}Pu. At the same time he consulted with Leal on ^{235}U, and later became a full participant in the work. In January of 1996, Leal, Derrien and 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 tailoring "external" resonances in each of the previous eleven regions. The evaluation covered eleven differential data sets (two fission and capture, one fission and absorption, six fission alone and two transmission). The new work matched the higher epithermal alpha and K1 of Release 6.3, and in addition provided excellent detailed fits to the differential data. It did well on the thermal benchmarks and produced better (lower) eigenvalues for the three intermediate-spectrum HISS (HUG) and UH3 cores.

However, M.C. Moxon [18] observed that the radiation widths fluctuated more than was expected theoretically. Moxon 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 resonances.

2.7 Leal-Derrien-Wright-Moxon – March 1997

To help resolve these questions, NEA, the UK and LMC jointly sponsored Moxon in a two-month visit to ORNL in late 1996. He and N.M. Larson worked to reconcile numerical and procedural differences between Moxon's code

REFIT [19,20] and SAMMY. All numerical constants were made consistent. Detailed comparisons among SAMMY, REFIT, NJOY and other codes led to a more accurate treatment of the low-energy free-gas model for Doppler broadening in REFIT [21]. Despite the validity of Moxon's observation that crystalline-binding models provide a better description of low-energy Doppler broadening than a free-gas, the effect is probably more important for ^{238}U than for ^{235}U, for which larger effects are still not adequately understood. Since crystalline-broadening is not yet available in ENDF-processing codes, practical considerations made it desirable to continue the work with the free-gas model. The width fluctuations were reduced in subsequent SAMMY fits by constraining the search region. During Moxon's stay at Oak Ridge, Leal, Derrien and Moxon, together with J.A. Harvey and R. Spencer of ORNL and M.S. Moore of LANL, were able to answer most questions regarding the ORNL experimental data-reduction procedures, e.g. ORNL confirmed that the target backings had been properly treated.

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 synthesised 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 harmonisation of the two codes. It should be emphasised, however, that the existence of two such sophisticated analysis tools and the expertise which their authors and users have brought to bear on the ^{235}U cross-sections, have resulted in higher-quality fits than was possible as recently as five years ago.

The resulting data set was benchmark-tested by Dean, *et al*. [22] and in the US by R.Q. Wright, A.C. Kahler and J.P. Weinman. The consensus was that the differential and integral characteristics were reasonable, but the evaluators felt that more could (and 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 Working Party on International Evaluation Co-operation (WPEC). The generation of this set utilised a new capability in SAMMY, allowing the inclusion of integral data (resonance integrals and 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 normalisation and background from the 1966 de Saussure capture and fission data [23] 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 be made before the October 1997 CSEWG meeting. That turned out not to be possible, and the two evaluation efforts are still separate.

In Moxon's data set a relatively low Maxwellian-averaged fission 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*. [24], which have already been adopted by both the Joint European File (JEF) and the Japanese Evaluated Nuclear Data Library (JENDL). A "hybrid" data set, created by inserting Moxon's cross-sections from 0-10 eV into the January 1996 ORNL evaluation and replacing the nubar file with the JEF values, was benchmark tested and performed satisfactorily on the thermal benchmarks. However, it did poorly on the harder-spectrum cases. Whether this is a low-α or a high nubar problem is not known. Another 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 (ENDF/B-VI Release 6.5)

After the WPEC meeting at Cadarache, ORNL and Moxon continued to refine their fits, and in August 1997 a new Leal-Derrien-Wright-Larson (LDWL) 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 6.3 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. A task for the future is to provide a less ad hoc solution to this problem. The radiation widths in the new LDWL 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 continuous-energy Monte Carlo 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 [25]. The best results were obtained using a reduced hydrogen capture cross-section, 332.0 mb instead of 332.6, as recommended by Kahler, and a version of oxygen that was slightly-modified from the Los Alamos evaluation in ENDF/B-VI Release 6.0 [26]. The effect of reducing the hydrogen capture was to raise the low-leakage end of the thermal benchmark "trend line" about 100 pcm. The modified oxygen has more forward scattering and the resulting additional 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 6.3, while the three harder cores are better, although not quite as close to unity as with the January 1996 evaluation of Leal-Derrien-Wright. In view of its good differential fits and benchmark performance, it was accepted for inclusion in ENDF/B-VI Release 6.5 (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 and P.G. Young.

In December of 1997, two papers were presented at a meeting of the JEF Working Group on Data Evaluation and Benchmark Testing [27,28]. Both showed significant improvements using LDWL over the JEF2.2 data set, which is similar to ENDF/B-VI Release 6.2. The studies covered a wide range of quantities, among them buckling measurements, k-infinities, spent-fuel analyses, and temperature dependent Westcott g-factors. In each area the LDWL 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 favourable findings, the new data were adopted for JEFF3.

Complete details of the LDWL evaluation were given in an ORNL report [29] and a slightly abbreviated version in the open literature [30]. Details of the inclusion of integral quantities into the analysis were also published as an ORNL report [31] and in the open literature [32].

2.11 Moxon – September 1997

Moxon has released a version of his latest work to the Nuclear Energy Agency Data Bank in Paris [33]. 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 earlier works [34]. 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 utilises 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 extent to which successive releases of ENDF/B-VI agreed or disagreed with integral benchmarks has from the start been an essential element in shaping its development. With the evolution of Release 6.3 and subsequent refinements, and the enhanced degree of international co-operation resulting from the formation of Subgroup 18, 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 LMC, A.C. Kahler and J.P. Weinman continuously monitored 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 (Lousiana State University) and R.D. McKnight (Argonne National Laboratory). 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 [35] under J. Blair Briggs (Idaho National Energy Laboratory) 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 [22,27,28,37-39]. 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.

Since there are 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}U evaluation

The current ENDF/B-VI evaluation (Release 6.5) [29,30] reaches some important goals:

1. The problems with the capture cross-section in the earliest releases are understood, at least for the thermal benchmarks:

    a. An average capture width of 38.03±1.70 meV in the range from 0 to 50 eV was obtained from the SAMMY analysis of a large set of experimental differential data, based on well-resolved time-of-flight experiments [39]. This agrees with the value (38.20±1.24) originally obtained by M.C. Moxon from an analysis of selected resonances in 0-20 eV [34], and with the value (38.2) obtained independently in Release 6.3 (0-100 eV) by adjusting the Release 6.2 capture cross-section upwards to match the bin-averaged capture of [5].

    b. The average capture width increased to 39.4±2.0 (+3.6%) when integral data were added to the experimental database [39]. This value agrees with the above to within the uncertainties.

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

    d. The capture widths, which were constrained in the fitting process, still show fluctuations of the order of 10%. This is considered to be acceptable in order to provide the best possible fit to the differential data. Moxon arrived at an alternative fit using a fixed value of the radiation width, achieving comparable χ^2 (goodness-of-fit) values, but at present there is no evidence indicating a technological difference between the two approaches. The point to be taken from these works is that one cannot expect a straightforward fit to the differential data to produce correct radiation widths. A value obtained some other way has to be imposed on the least-squares procedure.

2. Combining the resonance parameters into one region eliminated the

discontinuities between the eleven sub-regions in previous ENDF/B-VI releases, and simplified the representation of the distant level contribution.

3. The ORNL evaluation [40] reproduces below 0.1 eV the shape of η proposed by Santamarina, *et al*. [12]. The Gwin 1997 η data are well reproduced in the energy range below 1 eV, as discussed in [30]. The only problem is with the Wartena, *et al*. data [41] 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 LDLW 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 parameterised 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 the Reich-Moore formalism instead of Single-Level Breit-Wigner (SLBW) and incorporating the very accurate total cross-section obtained from Harvey's transmission data [42]; this could modify the fission and/or the capture cross-sections by a few per cent. A preliminary multilevel fit has been carried out by Moxon and shows a significant increase in α relative to an SLBW treatment [43]. Similar work is in progress at ORNL.

3. The ENDF/B-VI fission standard should be reconsidered [44]. If this standard is retained with its claimed accuracy, then the inconsistency between it and the ENDF/B-VI Release 6.5 evaluation will remain to be resolved, and will show up in the unresolved resonance region.

The current standard is based on the alpha measurements of Corvi, *et al*. [45] and of Muradyan, *et al*. [46]; the important data of Beer and Käppeler [47] obtained at Karlsruhe with a very high resolution were not considered. These data, in excellent agreement with the de Saussure, *et al*. data [48], are 6-7% 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 Harvey value.

4. Possible variation of nubar in the resonances was not considered in the ORNL (Release 6.5) 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 [24, 49-53]. The current good fits to the 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 α and η 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}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 discussed 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 organisations. First priority should go to the publication of new highly enriched, homogeneous benchmarks.

8. The question of over-absorption in ^{238}U continues to cloud benchmark results for low-enriched ^{235}U. Modern computational techniques, most importantly continuous-energy Monte Carlo calculations, could settle the issue of whether the basic data are responsible, or whether the

problem is in the reduction to multi-group cross-sections and related calculational approximations. To reach this goal, it would be desirable to first ensure an adequate degree of consistency among the various codes, so that calculational differences could be reliably ascribed to the basic data.

5. Conclusions

An extensive effort has gone into the evaluation and testing of the ^{235}U resonance region since the start of ENDF/B-VI in 1990. In Release 6.5 we 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}U cross-sections in low-enriched benchmarks.

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TABLES
AND FIGURES

Table 1. Thermal cross-sections and other parameters for some ^{235}U evaluations

Version	SIGC	GCAP	MAXC	SIGF	GFISS	MAXF	NUBAR	K1	RIC	RIF	EPITH. ALPHA
Standards	99.0	.9902	98.0	584.3	.9771	570.9	2.4320	719.5	–	–	–
ENDF/B-VI.1/2 (1)	98.8	.9895	97.8	584.5	.9786	571.9	2.4320	721.2	133.5	279.1	.478
ENDF/B-VI.3/4 (2)	98.6	.9897	97.6	584.8	.9786	572.3	2.4338	723.0	143.5	277.6	.517
LDW 1/96	98.8	.9888	97.7	584.5	.9790	572.3	2.4320	721.8			
LDWM 3/97	99.0	.9913	98.1	584.5	.9797	572.6	2.4338	722.9	139.8	276.8	.505
LDW 5/97	98.1	.9883	97.0	584.5	.9776	571.4	2.4338	722.3			
MOXON 5/97 (3)	99.5	.9507	94.6	581.6	.9771	568.3	(2.4338) (2.4374)	(720.2) (722.3)			
ENDF/B-VI.5 LDWL 8/97	98.7	.9911	97.8	585.0	.9765	571.3	2.4367	722.9	140.5	276.0	.509
MOXON 9/97	98.3	.9546	94.0	581.7	.9771	572.3	–	–	–	–	–

Notes: (1) ENDF6.2 did not change the cross-sections.
(2) ENDF6.4 corrected an error in the prompt nubar file in Release 3.
(3) The nubar values are not part of the evaluation, but are "representative" values. 2.4374 is JEF-2.2.

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.

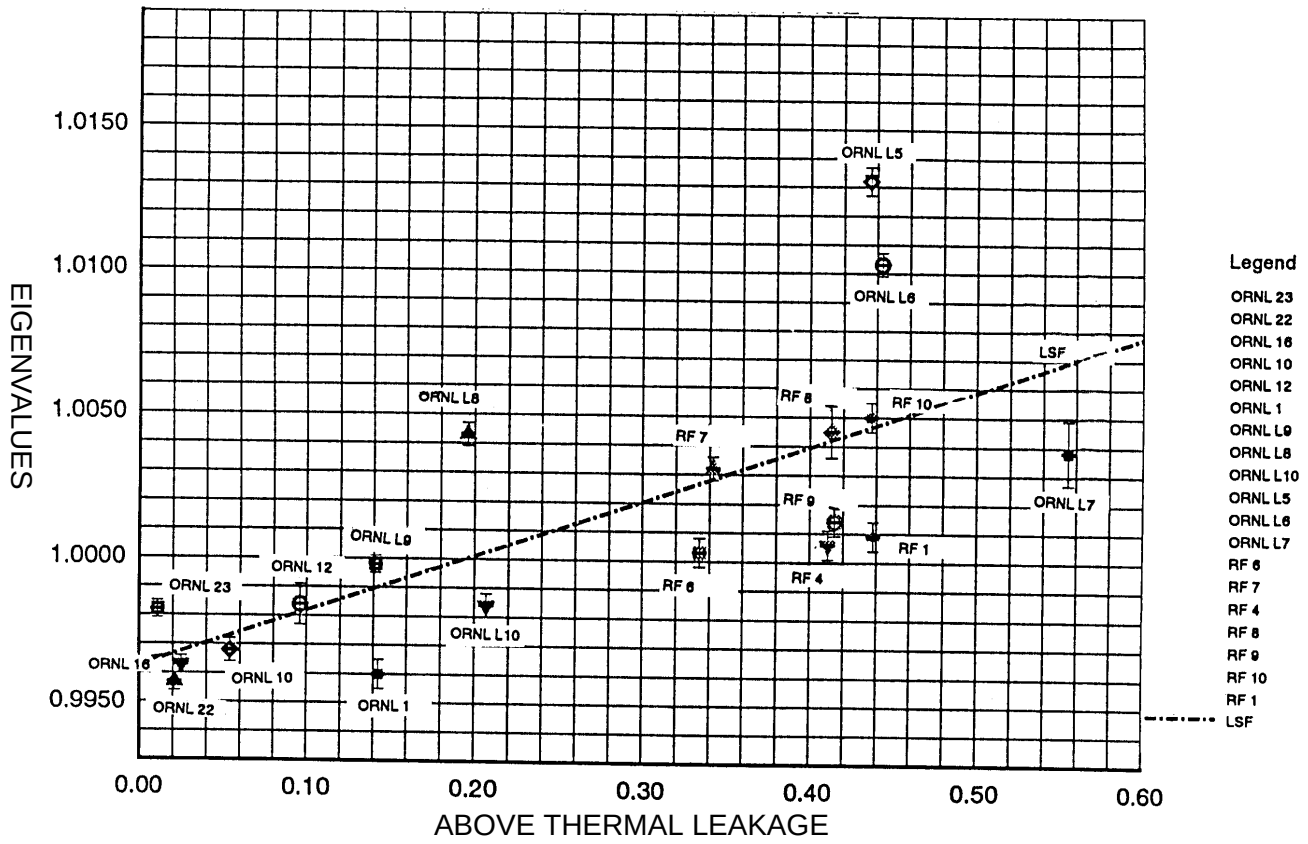

Figure 2. Eigenvalues of homogeneous critical assemblies vs. leakage (Oak Ridge and Rocky Flats). Calculated by continuous-energy Monte Carlo, using ENDF/B-VI Release 5 cross-sections.

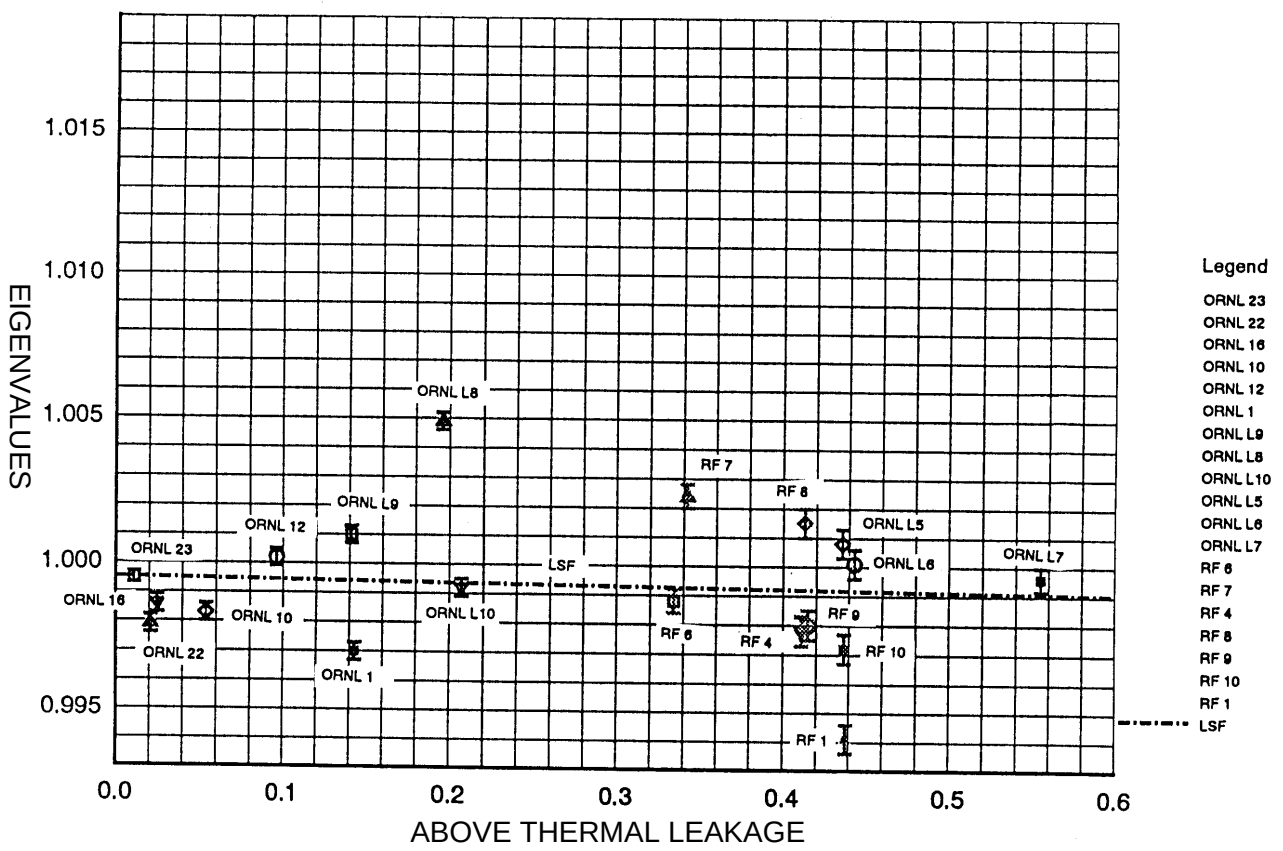

Figure 3. A comparison of the fission cross-section below 1 eV from ENDF/B-VI.5 and Moxon

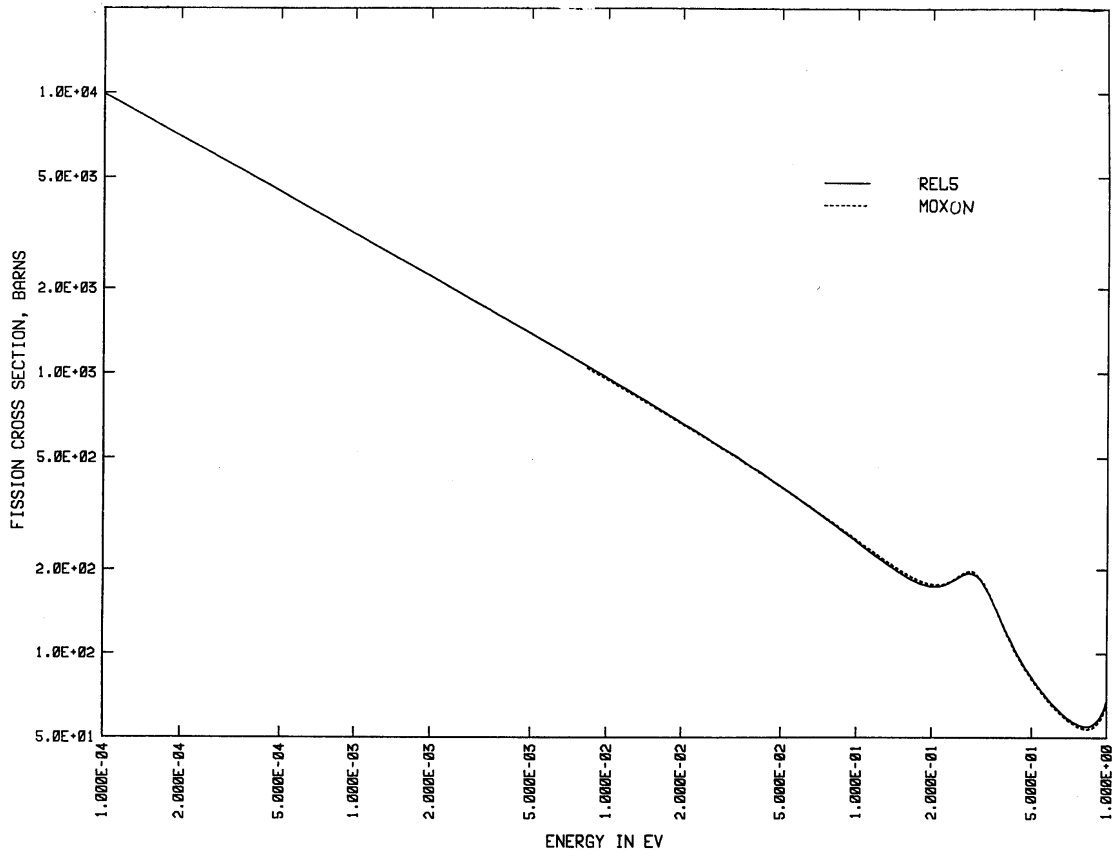

Figure 4. A comparison of the capture cross-section below 1 eV from ENDF/B-VI.5 and Moxon