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NUCLEAR DATA FOR IMPROVED LEU-LWR REACTIVITY PREDICTIONS

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 the 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 the goal of assessing and improving the quality and completeness of evaluated data.

The parties to the project are ENDF (United States), JEFF/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, is organised through the Nuclear Data Section of the International Atomic Energy Agency (IAEA).

The working party formed a subgroup to investigate a systematic reactivity under-prediction of thermal light water reactors fuelled with low-enriched uranium. The k_{eff} discrepancy (~ -500 pcm) was demonstrated with accurate Monte Carlo transport codes and the most recent nuclear data libraries (ENDF/B-VI.8, JENDL-3.3 and JEFF-3.0) available at that time. This report presents the trends given by the analysis of relevant integral experiments as well as the evaluation work, which focused mainly on ^{238}U nuclear data. During the course of this work, new evaluations of ^{238}U thermal capture cross-section, resonance parameters and inelastic scattering data were performed and provide a satisfactory solution of the problem. Finally, other nuclear data impacting the k_{eff} of thermal benchmarks, such as $^{16}O(n,\alpha)$ cross-section and ^{1}H-H_2O thermal scattering data, were also examined.

The opinions expressed in this report are those of the authors only and do not 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 22 was conceived to investigate a systematic reactivity under-prediction of thermal LEU-LWR (low-enriched uranium, light water reactor). This k_{eff} discrepancy (~ -500 pcm) was demonstrated with accurate Monte Carlo transport codes and the latest nuclear data libraries (ENDF/B-VI.8, JENDL-3.3 and JEFF-3.0) available in 2002. This report presents the trends given by the analysis of relevant integral experiments as well as the evaluation work, mainly focused on ^{238}U nuclear data. New evaluations of the ^{238}U thermal capture cross-section, resolved and unresolved resonance parameters and inelastic scattering data were performed and provide a credible solution to the problem. Reduced capture in the resolved resonances and a softer secondary inelastic scattering spectrum contributed about equally to the increased reactivity of the new data set. The newer inelastic data are mainly the result of improved theoretical models and more accurate differential measurements, but the choice of resonance parameters, although the state of the art in fitting procedures required some reliance on the integral benchmark data for its final form.

Other nuclear data impacting the k_{eff} of thermal benchmarks were also examined, such as the $^{16}O(n,\alpha)$ reaction, which had been the subject of discussion for several years. Based on a review of recent differential measurements, that cross-section was reduced by an amount that is consistent with the integral indications. A summary of the latest work on ^{1}H-$H_{2}0$ thermal scattering data is also given. The end result of these changes is an average eigenvalue over a broad class of assemblies which is close to unity.

NUCLEAR DATA FOR IMPROVED LEU-LWR REACTIVITY PREDICTIONS

1. Introduction

In the framework of the Working Party on International Nuclear Data Evaluation and Co-operation (WPEC), Subgroup 22 was initiated in 2002 with the objective to solve a discrepancy between the experimental and calculated k_{eff} of thermal LEU-LWR (low-enriched uranium, light-water reactor). A significant k_{eff} under-prediction (~ -500 pcm) was reported with the most recent nuclear data libraries available in 2002: ENDF/B-VI.8, JENDL-3.3 and JEFF-3.0.

The two characteristics of those data sets which led to the under-prediction were an over-absorption in the resonance region and a too-hard inelastic secondary spectrum. Although those characteristics had been present for many years, they were partially compensated by a too-low resonance capture cross-section in the early releases of ^{235}U evaluations. When Subgroup 18 [1] issued a revised ^{235}U data set that produced good agreement for the high-enriched uranium (HEU) benchmarks, it exacerbated the under-prediction for LEU.

Initially, there were some questions as to whether the Subgroup 18 work on ^{235}U was correct, but the satisfactory conclusion to Subgroup 22's work on ^{238}U suggests that the combination of the two data files is reasonable. Both data sets were developed with strong reliance on integral benchmarks, which we recognise does not produce unique results. The quantity and quality of the criticality benchmark database resulting from the work of the International Criticality Safety Benchmark Experiment Project (ICSBEP), however, makes this reliance less risky than at any previous time.

This report reviews the analysis of relevant integral measurements as well as the nuclear data evaluation work performed at several laboratories, mainly at the following:

- Oak Ridge National Laboratory (ORNL);
- Los Alamos National Laboratory (LANL);
- Commissariat a l'énergie atomique (CEA);

- International Atomic Energy Agency (IAEA);
- Knolls Atomic Power Laboratory (KAPL);
- Bettis Atomic Power Laboratory (BAPL);
- Nuclear Research and Consultancy Group NRG-Petten;
- Japan Atomic Energy Research Institute (JAERI);
- Westinghouse USA.

Communication within the group was efficiently carried out through a NEA mailing list "**ueval**" (**u**ranium **eval**uation) which allowed the group to function without face-to-face meetings. Archives of the discussions can be found at http://www.nea.fr/lists/ueval.html. It is hoped that this report will reflect the strong interactions that have been established between nuclear data evaluators and reactor physicists to solve the problem.

2. Statement of the problem

Before Subgroup 22 was set up, several benchmarking studies using continuous-energy Monte Carlo (CEMC) had raised the issue of LEU reactivity underestimation [2,3]. The problem was reported after extensive integral testing of the ^{235}U evaluation of the resolved resonances by the ORNL group [4], adopted in ENDF/B-VI.8, JEFF-3.0 and JENDL-3.3.

A description of the work on ^{235}U resonance parameters by ORNL and alternative fits by M. Moxon can be found in the final report of the WPEC Subgroup 18 [1]. It was shown that the latest ORNL ^{235}U evaluation, featuring a significant increase of the ^{235}U capture resonance integral, improves the prediction of k_{eff} of HEU systems and corrects the longstanding underestimation of ^{236}U build-up measured in pressurised water reactors (PWRs) (see for instance, papers by Chabert, *et al*. [5]).

Further studies by Kahler [6] and Weinman, *et al*. [7], involving benchmarks from the ICSBEP handbook and the Cross-section Evaluation Working Group (CSEWG) benchmarks book confirmed the problem with the newest nuclear data libraries available in 2002. ENDF/B-VI.8 produced the lowest values at around -700 pcm.

The under-prediction was reported for a large set of independent integral experiments performed at various laboratories and using different experimental methods to measure criticality (variation of moderator height, control rod adjustment, critical boron technique, etc.). It was therefore assumed that the k_{eff} discrepancy was not due to common experimental error. Since independent Monte Carlo codes and processing methodologies were used, it was also assumed that the problem was not the consequence of approximations or errors in transport computer codes.

The subgroup activities therefore focused on the analysis and re-evaluation of nuclear data impacting the k_{eff} of thermal lattices. The isotopes under investigation were ^{235}U, ^{238}U, ^{16}O and H_2O. However, given the extensive work devoted to ^{235}U in the resonance range and the good performance of the latest files for HEU benchmarks and post-irradiation experiments (PIE), the work concentrated on ^{238}U and, to a lesser extent, on ^{16}O and H_2O.

3. Analysis of ^{238}U integral trends

The resonance parameters of ^{238}U below 10 keV are the same in ENDF/B-VI.8, JEFF-3.0 and JENDL-3.3 and result from the work of a previous ^{238}U task force. The evaluation work performed at that time is summarised in the final report by M. Moxon and M. Sowerby [8].

The first task undertaken by Subgroup 22 was to analyse integral experiments sensitive to ^{238}U capture in order to test the accuracy of the Moxon resonance parameters and suggest trends to nuclear data evaluators. Several types of integral measurements were studied.

1. The k_{eff} bias was analysed as a function of ^{238}U capture fraction[1] [6,7]. The computations presented at the 2003 CSEWG meeting show a clear trend of decreasing k_{eff} with increasing ^{238}U capture fraction as illustrated in Figure 1. This striking correlation was interpreted as an overestimation of the ^{238}U capture shielded resonance integral (SRI). However, similar trends with other integral parameters such as the above thermal fission fraction (ATFF) [6] or the ^{235}U capture and fission fraction [9] were reported. Hence, it was argued that the observed trends might be attributable not only to ^{238}U but also to ^{235}U cross-section deficiencies.

2. Experimental ^{238}U spectral indices $\sigma_c^{238U}/\sigma_f^{235U}$ and the modified conversion ratio C^{U238}/F_{tot} provide relevant information on the accuracy of ^{238}U capture. The CEA-Cadarache team performed a detailed analysis of spectral indices measured at the EOLE facility [10] with JEF-2.2 (using the Moxon resonance parameters for ^{238}U). As illustrated in

[1] Ratio of ^{238}U capture rate over total absorption rate.

Table 1, the calculations, performed with the TRIPOLI4 Monte Carlo code (with a small statistical uncertainty), showed that the calculated ^{238}U capture rate was systematically overestimated by about 1.5 ± 1.0%.

Recent measurements of $^{28}\rho$ (ratio of epithermal to thermal neutron capture in ^{238}U) were performed at the Brazilian IPEN/MB01 and reported at the Santa Fe nuclear data conference in 2004 [11]. Computations using ENDF/B-VI.5 data slightly under-predict $^{28}\rho$.

MCNP calculations with JEFF-3.0 (Moxon's evaluation for ^{238}U) [12] of the DIMPLE benchmark gave (C-E)/E = 3.1 ± 1.9% for C^{U238}/F^{U235}, but the uncertainty of the Monte Carlo calculations was too high for conclusions to be drawn. Other studies involving older benchmarks such as TRX, compiled in the CSEWG benchmark book, also did not provide decisive evidence for ^{238}U capture overestimation.

Figure 1. Calculated eigenvalues of 17 configurations of the Leu-Comp-Therm-006 benchmark, plotted as a function of ^{238}U capture fraction, using ^{238}U cross-sections from ENDF/B-VI.5 and a new evaluation presented in Section 4

Calculations by J.P. Weinman, et al. [7] with the RACER Monte Carlo Code

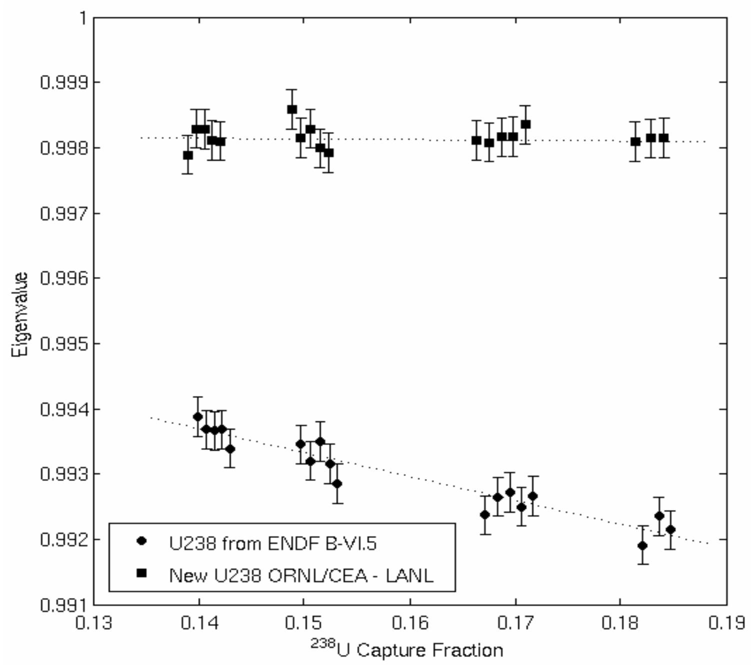


Table 1. Comparison between calculated and measured values of spectral indices for several thermal lattice experiments performed at CEA-Cadarache, as published in PHYSOR-2000 [10]

Experiment name, fuel type	Spectral index	(C-E)/E	Experimental uncertainty
Mistral-1 UO_2	C^{U238}/F_{tot}	+2.2%	±2.0%
Mistral-2 UO_2-PuO_2	C^{U238}/F_{tot}	+2.3%	±1.5%
Erasme-S UO_2-PuO_2	$\sigma_c^{238U}/\sigma_f^{235U}$	+1.6%	±2.3%
Erasme-R UO_2-PuO_2	$\sigma_c^{238U}/\sigma_f^{235U}$	-0.2%	±2.1%

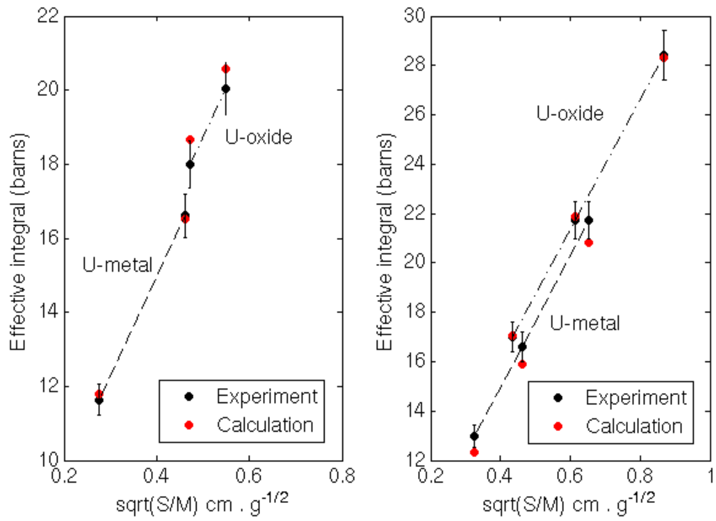
3. A series of experiments performed in the late 1950s and early 1960s used an activation technique to measure the ^{238}U capture rate of isolated fuel rods of various compositions (UO_2 and U metal) and geometries. These experiments were carefully reviewed by Eric Hellstrand in 1966 [13], and recommended values of the ^{238}U effective resonance integral were tabulated as a function of surface-to-mass ratio of the rod $\sqrt{S/M}$ using the following empirical formula: $I_{eff} = a + b\sqrt{S/M}$. The results, known as the "Hellstrand correlations" were revisited in different ways. The first methodology (A. Courcelle and A. Santamarina at CEA-Cadarache [14], H. Huriah at Westinghouse [15], consisted of defining an idealised pin-cell benchmark, in which the computed SRI can be directly compared with the Hellstrand correlations values. In the second study by D. Hanlon and C. Dean [16], a specific experiment performed by Hellstrand and his collaborators [17] in the R1 reactor at Stockholm was modelled in detail with the Monte Carlo code MONK.

   Initially, it was believed that these experimental data would help decide the issue, but because of the large experimental uncertainties, it was concluded that the Hellstrand correlations were not sufficiently accurate to draw firm conclusions (see Figure 2). According to Hellstrand himself, "limits of error below 3.5% (on ^{238}U capture SRI) could scarcely be obtained".

4. Measurements of ^{239}Pu production versus burn-up in post-irradiation experiments (PIE) are also a valuable check of the ^{238}U capture SRI. In the French experiments with UO_2 fuel, CEA computations with JEF-2.2 indicated that the ^{239}Pu/^{238}U isotopic ratio was systematically overestimated by 1 to 3% depending on the experimental configuration and burn-up [5,10,18]. Again, this discrepancy is in the uncertainty range of the experiments but supports a ^{238}U SRI decrease of about 0.5-1.5%. Adjustment studies based on PIE results [18,19] confirmed this estimate.

Figure 2. Comparison of calculated and experimental values of the ^{238}U effective resonance integral

The left figure summarises the results of Hanlon, et al. [16] who investigated one measurement performed in the R1 reactor at Stockholm [17]. The figure on the right shows the comparison between Monte Carlo calculations by Courcelle [14] and Huriah, et al. [15] and the compilation of four measurements by Hellstrand [13]. In all cases, the resonance parameters of Moxon [8] were used.



In the above four categories, only a limited number of experiments were investigated and a broader set would be needed to provide more accurate conclusions on ^{238}U capture. In themselves, these findings do not demonstrate a significant problem with the ^{238}U evaluation of Moxon, since they lie within the uncertainty margins (3σ) of the integral measurements. Nevertheless, they suggest a small decrease of the ^{238}U effective capture resonance integral by about 1%. This estimate is considered to be within the experimental uncertainty of both present-day integral and differential measurements. Given the high sensitivity of the reactivity of uranium-fuelled systems to ^{238}U capture, the proposed modification would eliminate the decreasing trend of k_{eff} bias with increasing ^{238}U capture fraction and improve the k_{eff} prediction.

4. ^{238}U evaluation work

4.1 Thermal capture cross-section

In a typical thermal light water UO_2 lattice, approximately 20% of the ^{238}U captures occur below 4 eV. Therefore, it was appropriate to review the accuracy of the ^{238}U thermal capture cross-section, especially considering that discrepant recommendations were provided in the open literature:

- σ_0 = 2.708 b (from the CSEWG Standards Committee);
- σ_0 = 2.718 b (from the resonance parameters of Moxon[2] [8];
- σ_0 = 2.680 ± 0.019 b (from the latest Mughabghab work [20]).

To investigate these differences, the $^{238}U(n,\gamma)$ thermal cross-section was reviewed in detail by A. Trkov and co-workers. A detailed description of the work was published in *Nuclear Science and Engineering* [21]. From an extensive review of the original publications, the published values were corrected for more recent standard cross-sections and other data used in the experimental analyses. In addition, a new activation measurement, performed by G. Molnar, *et al*. [22] at Budapest, was also investigated. Due to its importance in the experimental determination of the thermal $^{238}U(n,\gamma)$ through activation measurements, the gamma-ray emission probabilities from the β decay of ^{239}Np were also evaluated. The least-squares fit was performed with the ZOTT99 code in the log-domain to avoid Peele's Pertinent Puzzle, widely discussed in the field of standard cross-section evaluation. The final $^{238}U(n,\gamma)$ thermal value is as follows:

$$\sigma_0 = 2.683 \pm 0.012 \text{ b}$$

This value is 1.5% lower than in the JEFF, ENDF and JENDL evaluations based on Moxon's resonance parameters and consequently decreases slightly the calculated capture rate in thermal benchmarks. It was also concluded that most of the measurements were relatively old and that new measurements with accuracy better than 1% would be beneficial to confirm the present recommended value.

4.2 Adjusted cross-sections for sensitivity studies

Considering that the integral trends suggested a small reduction of the ^{238}U resonance capture cross-section, C.R. Lubitz (KAPL) made two different adjustments of the Moxon resonance parameters to assess the relative impact of changing radiation and neutron widths. The first consisted of a uniform reduction by 1.35% of the radiation widths of the s-wave positive-energy resonances, whereas the second lowered the neutron widths by 0.74%, leaving the radiation widths unaltered. The first of these numbers made the average

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2 A CSEWG recommendation to reduce this value to the Standards value was apparently never implemented in the ENDF file.

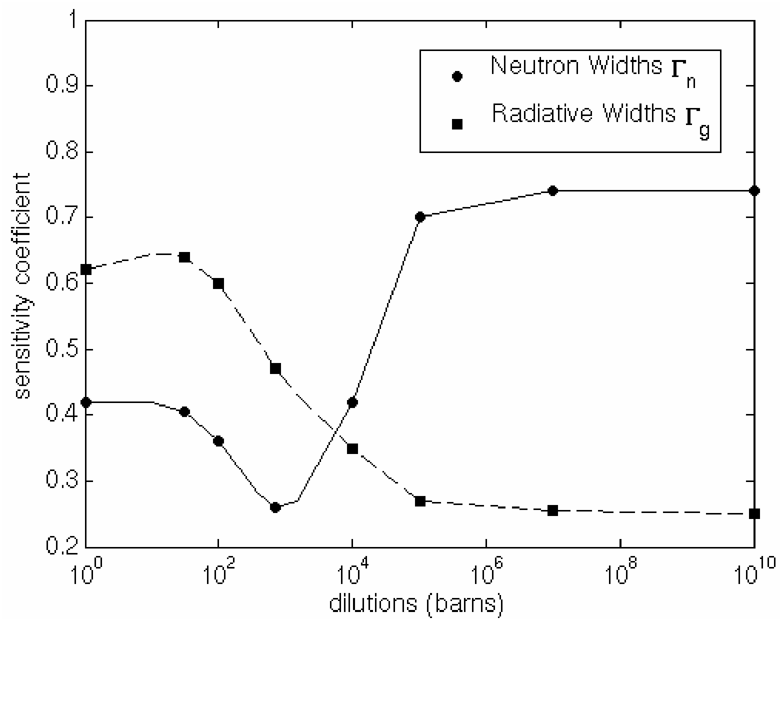
radiation width in the resolved resonance region agree with the slightly lower value determined by Fröhner [23] for the unresolved region. The second number was chosen so that both data sets had the same dilute capture resonance integral, 276.6 b. The effective radius was not modified and was 9.42 fm in both cases. Using the negative-energy resonances, the thermal capture cross-section was adjusted to 2.708 b in both adjustments. A similar approach was used to investigate the resonance range of ^{235}U [24].

The effect of these modified parameters on capture SRI and k_{eff} were, of course, not equivalent, the Γγ adjustments giving a higher effect (-0.7%) than Γn (-0.2%) on the SRI at dilution σ_d = 50 b. As expected, both sets improved the k_{eff} prediction of low-enriched thermal lattices.

Sensitivity coefficients of capture SRI to resonance parameters versus dilution, calculated by Mounier [18], are shown Figure 3, and corroborate the effect of the KAPL adjustment.

Figure 3. Sensitivity coefficients of the shielded capture resonance integral to a uniform change of the resonance parameters (Γγ and Γn) below 150 eV, as a function of dilution (from Mounier, *et al*. [18])

This figure shows the high sensitivity of the capture SRI to Γγ in the dilution range typical of LWR (20-100 b)



4.3 Resolved resonance parameters

A new evaluation of ^{238}U resonance parameters was performed at ORNL in collaboration with CEA-Cadarache. This work was motivated not only by the reactivity prediction problem, but also by the possibility of improving the resonance parameters with previously unanalysed differential measurements. A full account of the work is available in Ref. [25], in an ORNL report [26], and will be submitted for publication in *Nuclear Science and Engineering*.

The experimental database used in the evaluation is presented in Table 2. The data were analysed with the Bayesian Reich-Moore code SAMMY [27]. Compared with previous work, the ORNL/CEA evaluation benefited from the high-resolution transmission measurements [28], from 1 to 100 keV, performed by Harvey, *et al*. at the Oak Ridge Electron Linear Accelerator (ORELA, see Figure 6). The capture data of Macklin [29], partially analysed by Moxon in the previous ^{238}U task force [8], were fully included in the fit. The capture data performed at Harwell by Moxon, *et al*. [30], valuable for the evaluation of resonance parameters below 100 eV, were unfortunately not available.

Table 2. Main differential experiments used in the SAMMY analysis of ^{238}U resonance parameters

Other measurements were analysed (subthreshold fission and thick transmission measurements for p-wave resonances) but are not quoted in this table

Energy range of analysis	Reference	Measurement type
Thermal range	Corvi, *et al*. [31]	Capture
6-38 eV	Meister, *et al*. [32]	Transmission
6-10 keV	de Saussure, *et al*. [33]	Capture
0.5-4 keV	Olsen, *et al*. [34]	Transmission
300 eV-10 keV	Olsen, *et al*. [35]	Transmission
1 keV-20 keV	Harvey, *et al*. [28]	Transmission
250 eV-20 keV	Macklin, *et al*. [29]	Capture

Most of the conclusions drawn in the previous ^{238}U task force were confirmed by the new ORNL/CEA work. In particular, sequential fits of capture data along with transmission data detected significant errors in normalisation in the capture data: ~ -10% in the de Saussure, *et al*. data above 100 eV and ~ +15% in the Macklin, *et al*. data. In addition to normalisation errors, the SAMMY fit suggested that a constant background cross-section of about 50 mb for de Saussure and 110 mb for Macklin should be subtracted. The existence of a direct capture component was at first suspected since the simple Lane-Lynn model [36] gives an estimate of 80 mb. However, more realistic calculations by

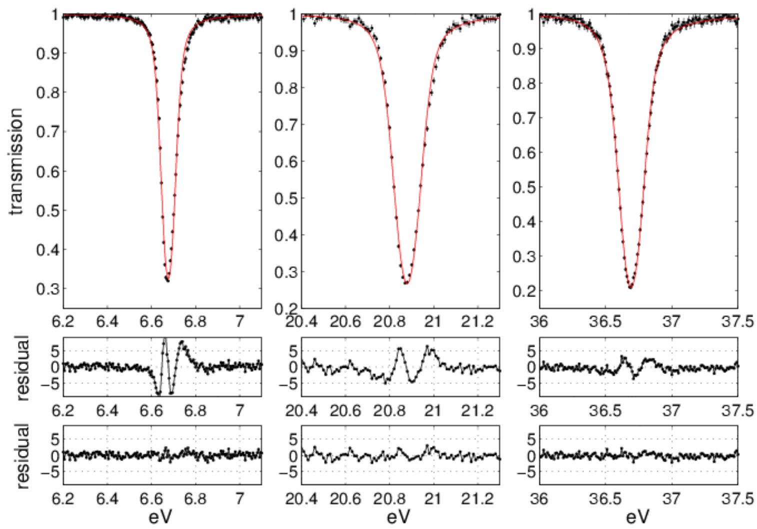
G. Arbanas [37] indicated that the direct and semi-direct capture cross-section should not exceed a few millibarns. The final resonance file is self-contained in File 2, no File 3 background being required.

The effective radius, which depends on the choice of external resonances, is 9.48 fm, close to the previous Moxon value of 9.43 fm. The thermal scattering cross-section was evaluated by compiling the measurements of coherent scattering length, and the value of σ_s = 9.28 b, which is lower than in Moxon's evaluation (σ_s = 9.38 b) was chosen. The ORNL/CEA evaluation adopted the recommendation described in the previous section for the ^{238}U(n,γ) thermal cross-section: σ_0 = 2.683 b (2.718 b in Moxon's evaluation).

Measurements of the large resonances at 6.67, 20.86 and 36.6 eV were carefully analysed with the Crystal Lattice Model (CLM) instead of the traditional, simpler Free Gas Model (FGM) with effective temperature for Doppler broadening. The CLM, first derived by W. Lamb [38] and newly implemented in the SAMMY code, accounts for the chemical binding between atoms in the U-oxide or U-metal samples. The CLM was experimentally validated with low-temperature transmission experiments performed by Meister, *et al*. [32] at GELINA (see Figure 4), and used for the final fit.

Figure 4. SAMMY fits of the UO_2 transmission data from Meister, *et al*. [32] measured at GELINA at low temperature (T = 23.7 K)

The middle figure displays the residual with the Free Gas Model with a fitted temperature; the bottom figure shows the improvement of the residual with the Crystal Lattice Model without any temperature adjustment [39]



At room temperature or higher, Doppler-broadened cross-sections reconstructed from the resonance parameters using either the CLM or the usual free-gas-at-ambient-temperature method, will be indistinguishable. However, the reduced capture resulting from the low-temperature CLM fitting is still significant.

As shown in Table 3, the ORNL/CEA final resonance parameters below 102 eV are fairly close to Moxon's. The average radiation width below 102 eV is 23.1 meV, consistent with the previous determination. The main difference is slightly lower neutron widths.

Table 3. ^{238}U resonance parameters below 102.5 eV from Moxon and the final version of the ORNL/CEA evaluation

Energy eV	Moxon Γγ meV	Moxon Γn meV	ORNL/CEA Γγ meV	ORNL/CEA Γn meV
6.674	23.00	1.493	23.00	1.476
20.87	22.91	10.26	22.86	10.09
36.68	22.89	34.13	23.00	33.55
66.03	23.36	24.60	23.31	24.18
80.75	23.00	1.865	23.39	1.874
102.5	23.42	71.70	24.08	70.77
Effective radius	R′ = 9.43 fm		R′ = 9.48 fm	

Figure 5. SAMMY fits of the three ^{238}U capture data sets available

Two samples from Macklin, et al. [29] and one sample from de Saussure, et al. [33]). Experimental data were significantly renormalised as explained in the text.

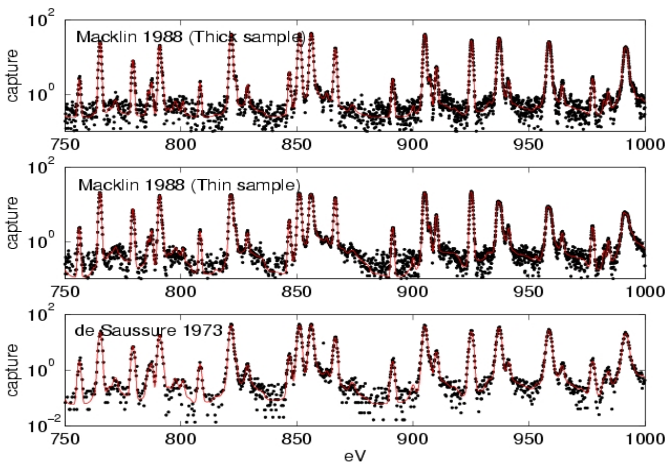
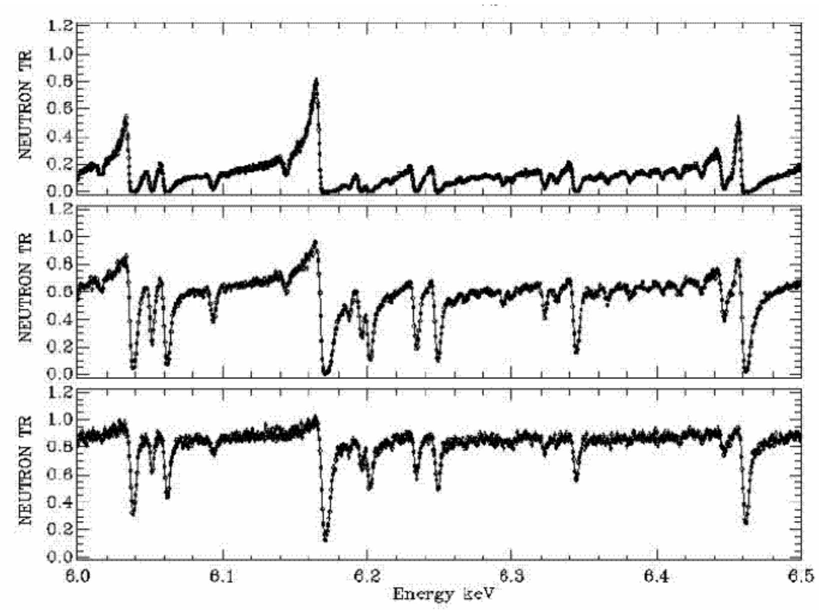


Figure 6. SAMMY fits of sample transmission data from Harvey, *et al*. [28] through ^{238}U sample thicknesses of 3.62, 0.250 and 0.083 cm, respectively, from the upper curve to the lower curve

Figure taken from [26]



The Harvey transmission and Macklin capture data allowed the extension of the resolved range from 10 keV to 20 keV. However, above 10 keV, the experimental resolution made the resonance analysis difficult such that even resonance energies could not be reliably determined. A "pseudo-resonance" approach was used; a set of resonances was statistically generated and modified to fit the structure of transmission and capture data but which does not represent actual resonances. Between 10 and 20 keV, the average capture cross-section derived from the new resolved resonance parameters is about 5% lower than the value deduced from Fröhner's [23] ENDF/B-VI.8 unresolved resonance parameters. More work is needed to understand this discrepancy.

Extensive statistical tests of the ORNL/CEA s-wave resonance parameters were performed by comparing the resonance data with the Gaussian-Orthogonal Ensemble predictions [40]. Reasonable agreement was found up to 3 keV for the s-wave resonances. The impact of the new resonance parameters on integral benchmarks is described in Section 5.1.

4.4 Unresolved resonance range

The capture cross-section in the unresolved resonance range above 20 keV is important for fast and intermediate-spectrum reactors (less so for thermal benchmarks) and has not received extensive testing by Subgroup 22. The capture cross-section was previously studied in the framework of Subgroup 4 [41], and new evaluations were subsequently released by Kawano, *et al*. [42] and Maslov [43]. Recent work includes the following:

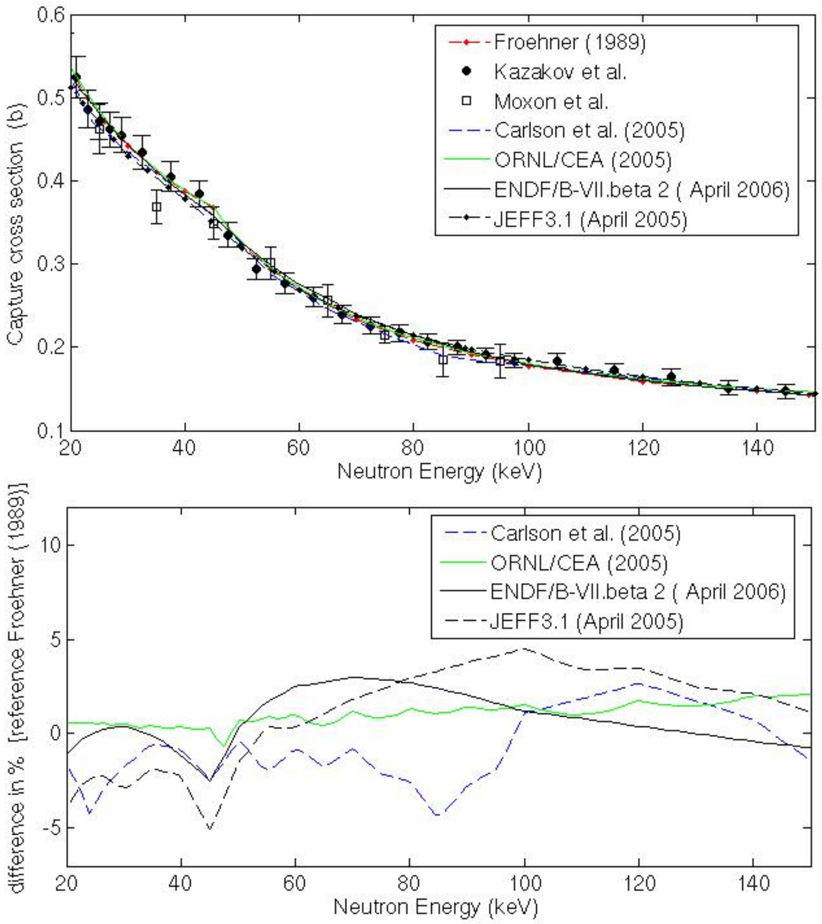
1. Above 20 keV, new coupled-channel calculations were performed by CEA/BRC [44] using the ECIS95 code and optical-model parameters based on the study of [45]. The capture cross-section was calculated with a modified version of the GNASH statistical code. This evaluation was adopted in File 3 of JEFF-3.1, along with average parameters from Fröhner [23] in File 2.

2. Following the work on the ^{238}U resolved-resonance parameters, a new analysis of the unresolved resonance range was also performed [40]. The work was based on the statistical model as implemented in SAMMY, adapted from Fröhner's FITACS code. Average parameters such as the neutron strength function, scattering radii and average radiative widths were not determined by nuclear models but were fitted to a comprehensive experimental transmission and capture database using starting values and uncertainties from a statistical analysis of s- and p-wave resolved resonances below 20 keV. This work benefited from the Harvey (ORELA) transmission data described in the previous section.

3. The CSEWG Standards Committee under A.D. Carlson produced a new evaluation of ^{238}U capture [46]. It is not an official standard but is rather a by-product of the standards evaluation process. Capture cross-section values are not based on nuclear models but are the result of simultaneous adjustment by the GMA code of a large experimental database containing absolute measurements, cross-section ratios, etc. After some smoothing and slight modifications, this evaluation was the basis of the preliminary ENDF/B-VII.β2 library (File 3) [47,48].

The last two analyses relied heavily on experimental data. As in Fröhner's work, the evaluated capture cross-section is based mainly on the measurements by Kazakov, *et al*. [49] and Moxon, *et al*. [30], whose normalisations are consistent. As shown in Figure 7, the newest evaluations of capture cross-section are close to Fröhner's and the small differences between them have little impact on the thermal benchmarks.

Figure 7. Comparison of recently evaluated ^{238}U capture cross-sections in the unresolved resonance range [40,46], ENDF/B-VII.β2 [47] and JEFF-3.1 [44] with the reference measurements of Kazakov, *et al*. [49], Moxon, *et al*. [30] and Fröhner's evaluation [23]. The lower figure shows the percentage difference with Fröhner's.



4.5 Inelastic scattering data

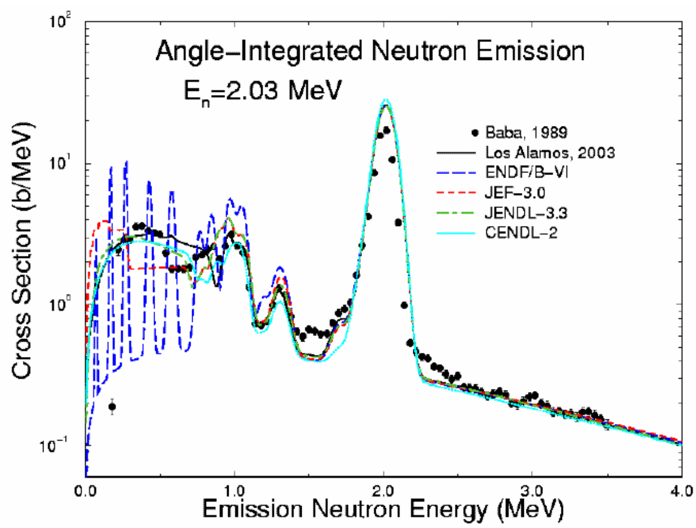
Over the past 20 years, extensive work has been devoted to the theoretical modelling of ^{238}U inelastic cross-sections. In 1989, WPEC Subgroup 4 [41] simulated a series of measurements on ^{238}U(n,n′) with the aim to resolve observed discrepancies and to reduce the uncertainties in previous data. Experimental neutron spectrum and partial inelastic cross-section measurements listed in Ref. [41] provided valuable insight.

In the meantime, coupled channel calculations were improved, as were statistical and pre-equilibrium models, leading to better predictions of the inelastic cross-section and secondary-neutron spectra. As a result of Subgroup 4 efforts, improved evaluations of ^{238}U inelastic data were produced by Maslov, *et al*. [43] and Kawano, *et al*. [42].

Recently, two independent evaluations by the LANL and BRC groups were undertaken and successive releases were distributed to Subgroup 22 for testing. This work was summarised at the Santa Fe conference by Young, *et al*. [47,48] and by Lopez-Jimenez, *et al*. [44]. Compared with the ENDF/B-VI.8 and JEF-2.2 evaluations, which predate Subgroup 4, the new models agree better with experimental data. Of particular interest are the spectra of secondary neutrons produced by inelastic scattering and fission, as measured by Baba, *et al*. [50] at different incident energies. As shown in Figure 8, the recent evaluations of double-differential cross-section are of better quality than in ENDF/BVI.8 or JEF-2.2.

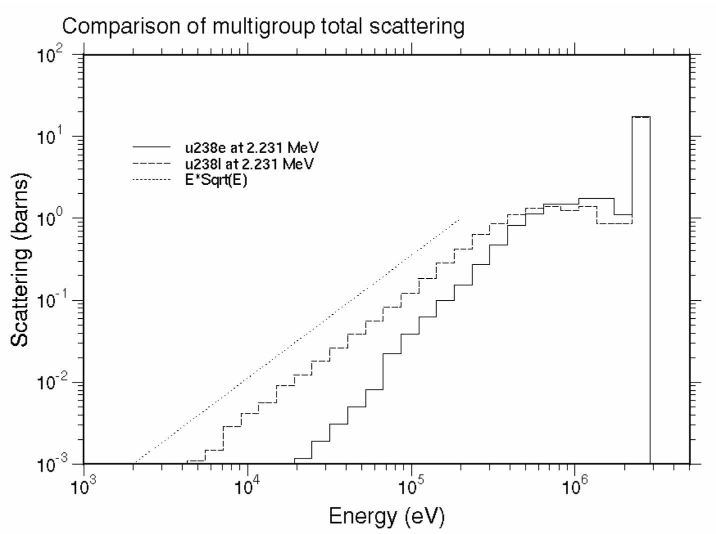
Figure 8. Comparison of angle-integrated neutron emission spectra (mainly fission and inelastic) from various evaluations with the measurement of Baba, *et al*. [50] at incident neutron energy En = 2.03 MeV

Figure from [48]



As displayed in Figure 9, the new evaluation features a softer inelastic secondary neutron spectrum compared with the previous one of ENDF/B-VI.8 or JEF-2.2. The influence of these new data on the smaller thermal benchmarks was found to be significant, increasing k_{eff} by reducing the neutron leakage, as explained in Section 5.

Figure 9. Comparison of multi-group transfer matrix at incident neutron energy of 2.231 MeV for preliminary evaluations performed at LANL (labelled as u238l) and the previous version in ENDF/B-VI.8 (u238e)



5. Integral tests of the new ^{238}U evaluations

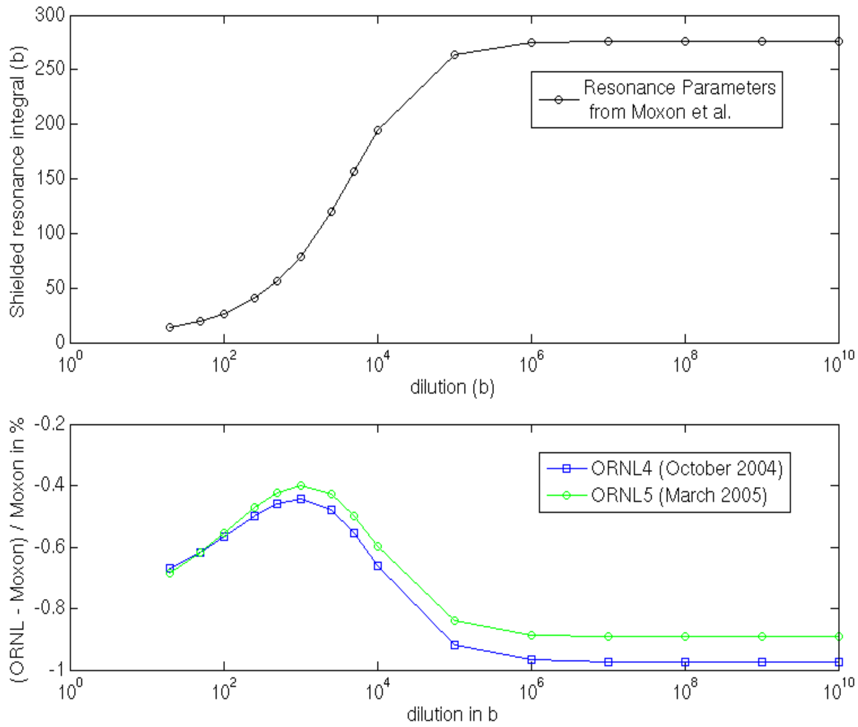
5.1 Effect of new resonance parameters

The new ^{238}U resonance parameters provide a lower capture cross-section both in the thermal and resonance ranges. The impact of these changes is easily assessed by computing the effective resonance integral for different dilution values under the infinite-medium assumption. As shown in Figure 10, the capture SRI is lowered by about 0.6% at 50 barns dilution with the new set of resonances.

In actual reactor calculations, the observed effect is a decrease of the calculated ^{238}U reaction rate and a corresponding increase of k_{eff} between 100 and 300 pcm depending on the moderation ratios. More importantly, the observed slope of k_{eff} bias versus ^{238}U capture is well corrected [7], as shown in Figure 1.

Figure 10. Comparison between the ^{238}U effective resonance integral (integration from 1.0 eV to 10 keV) of the ORNL/CEA and Moxon evaluations for various dilution values

ORNL4 is a preliminary version of the resonance parameters that were adopted in JEFF-3.1, while ORNL5 is the final version (adopted in the preliminary ENDF/B-VII.β2 library)



5.2 Substitution analysis

A powerful way to determine the importance of cross-section changes in benchmark calculations is reaction-substitution analysis. The idea is to substitute reaction by reaction the cross-section values from one evaluation into another and to perform benchmark calculations after each substitution. An illustration of this technique was presented by J. Weinman using the Leu-Comp-Therm-006 benchmark. The aim was to understand the large k_{eff} increase (about 600 pcm) between calculations with the new ^{238}U file and the previous ENDF/B-VI.5 evaluation. This study shows the importance of the new resonance parameters and the new inelastic transfer cross-section in the k_{eff} change (see Table 4). The transfer matrix is "normalised" so its effect is independent of changes in the

Table 4. Result of substitution analysis performed by J. Weinman to compare ENDF/B-VI.5 evaluation and the new ^{238}U file combining preliminary LANL and ORNL/CEA work. It shows the change in eigenvalue for each reaction and highlights the impact of the resonance parameters and inelastic transfer matrix.

Case description	k_{eff}	Unc. 2 σ	Change in k_{eff} relative to base case	Unc. 2 σ	Change in k_{eff} for reaction type	Unc. 2 σ
Base case: ENDF/B-VI.5	**0.99191**	**0.00032**				
Prev. case + inel. transfer	0.99465	0.00031	0.00274	0.00045	**0.00274**	0.00045
Prev. case + inel. xs	0.99413	0.00030	0.00022	0.00044	-0.00052	0.00043
Prev. case + elastic xs	0.99329	0.00033	0.00138	0.00046	-0.00085	0.00045
Prev.s case + el. moments	0.99376	0.00029	0.00185	0.00043	0.00047	0.00044
Prev. case + capture xs	0.99701	0.00032	0.00510	0.00045	**0.00325**	0.00043
Prev. case + fission xs	0.99762	0.00031	0.00057	0.00045	0.00062	0.00045
Base case + LANL/ORNL ^{238}U	0.99809	0.00030	0.00618	0.00044		

inelastic cross-section itself. The 47 pcm difference between the last two rows is due to the inconsistency inherent in changing resonance cross-sections for elastic scattering and capture separately.

5.3 Summary of k_{eff} benchmarking studies

The successive versions of the ORNL/CEA resolved range evaluation and the fast range data from LANL and BRC were merged into two complete ^{238}U test files. Within the working group, several CEMC codes were used:

- MCNP [51] (versions 4 and 5), developed at LANL;
- RCP [6], developed at BAPL;
- RACER [52], developed at KAPL;
- TRIPOLI4 [53], developed at CEA-Saclay;
- MONK8 [54], developed at SERCO Assurance.

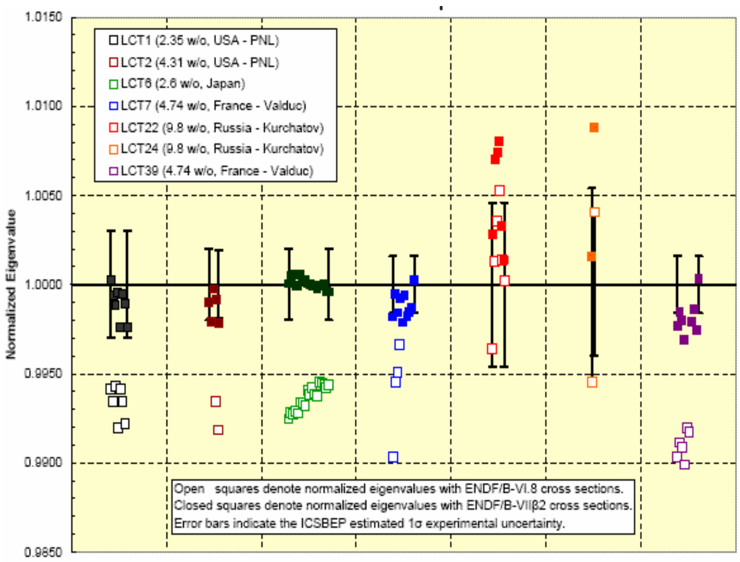
Subgroup 22 did not perform a rigorous comparison of these codes, but in most cases reasonably good consistency was found. Eigenvalue differences between TRIPOLI4 and MCNP up to 150 pcm for some Leu-Comp-Therm configurations were initially noticed, but were resolved by a closer comparison of the two codes. Code differences hinder analysis of cross-section effects at the 100 pcm level but did not preclude agreement that the combination of the ORNL/CEA resonances and the LANL/BRC inelastic data provided a satisfactory solution to the k_{eff} problem.

Integral testing, mainly by Weinman, Kahler, MacFarlane, van der Marck, Trkov and Sublet, demonstrated the improvement of the reactivity prediction for a large number of low-enriched thermal lattices. The paper presented by MacFarlane [55] at the 2004 Santa Fe nuclear data conference provides a good example of the performance of these files with MCNP5. More recent references are available in the form of JEFDOCs [56,57] or as contributions to the CSEWG meeting [58-60].

The most recent k_{eff} calculations (April 2006) were performed with JEFF-3.1 and ENDF/B-VII (β2 version), which includes the new ^{238}U files. An example of such calculations is presented in Figure 11. Benchmarking results are continuously posted on the CSEWG website[3] for the ENDF project, and on the JEFF website[4].

Figure 11. Calculated eigenvalues for Leu-Comp-Therm benchmarks with ENDF/B.VI.8 and ENDF/B-VII.β2 cross-section data sets

Calculations were performed at LANL by Kahler and MacFarlane with MCNP5



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3 http://www.nndc.bnl.gov/csewg/

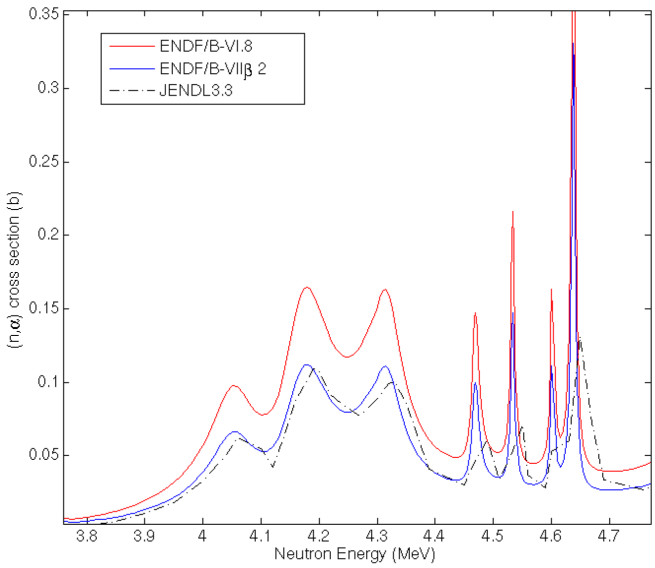
4 http://www.nea.fr/html/dbdata/projects/nds_jef.htm

6. Other nuclear data

6.1 Oxygen (n,α) cross-section

ENDF/B-VI.8 and JEFF-3.0 share the same evaluation based on the work of G. Hale [61] at LANL using the R-matrix EDA code. Recent R-matrix analysis of $^{16}O(n,\alpha)$ was also performed at ORNL with the SAMMY code by R. Sayer, *et al*. [62]. The $^{16}O(n,\alpha)$ cross-section in JENDL-3.3 is significantly lower than the other evaluations, as shown in Figure 12. This difference has a small but non-negligible impact of about 50 pcm on thermal reactor benchmarks (with UO_2 fuel and H_2O moderator).

Figure 12. Comparison of $^{16}O(n,\alpha)$ cross-section from ENDF/B-VI.8, JENDL-3.3 and the recent evaluation by Page, *et al*. [63] adopted in the preliminary ENDF/B-VII.β2 library



Experimentally, $^{16}O(n,\alpha)$ cross-sections are usually derived by reciprocity from the inverse reaction $^{13}C(\alpha,n)$. Despite the large number of experiments, most of them were performed with a rather poor energy (neutron or α) resolution. Values for $^{16}O(n,\alpha)$ from ORNL and LANL evaluations rely mainly on the measurements of Bair, *et al*. [64] and Drotleff, *et al*. [65]. The Bair, *et al*. publication suggests, in an added note in proof, to renormalise upward the original data. Regardless of how the Bair data are renormalised, they are still significantly higher than the Drotleff data (by about 10-20%) and higher than older data such as Sekharan, *et al*. [66] or Walton, *et al*. [67] (by 50%).

Subgroup 22 sent a request to the WPEC High Priority Request List to simulate a new measurement and solve this problem [68]. Fortunately, after further investigation, two recent measurements by Heil, *et al*. [69] and Harissopulos, *et al*. [70] were found. A detailed analysis of the two experiments is still needed to draw a solid conclusion on the $^{16}O(n,\alpha)$ cross-section, though a preliminary analysis supported a significant decrease of the $^{16}O(n,\alpha)$, placing the level of the cross-section close to that of JENDL.

Page, *et al*. at LANL [63] proposed a preliminary evaluation, displayed in Figure 12, and integral testing demonstrated the slight increase of k_{eff} of thermal lattices (about 30-40 pcm).

6.2 ^{235}U prompt-neutron fission spectrum

At the 2003 WPEC meeting in San Diego, D. Madland concluded the work of Subgroup 9 on the evaluation of fission neutron spectra. The final report [71] pointed out large discrepancies in the peak and tail regions between the two most recent measurements of the ^{235}U spectrum for thermal neutrons. The latest evaluation proposed by Madland was still preliminary, but was found to deteriorate the prediction of the Heu-Sol-Therm as well as Leu-Comp-Therm benchmarks and was not adopted in the latest versions of ENDF or JEFF.

Despite the work done at Los Alamos to understand the discrepancy and improve the theoretical modelling, a highly accurate measurement of the ^{235}U thermal fission spectrum is strongly needed.

6.3 H-H_2O cross-section and $S(\alpha,\beta,T)$[5]

The subgroup initially targeted the hydrogen-in-water cross-section for investigation for three reasons:

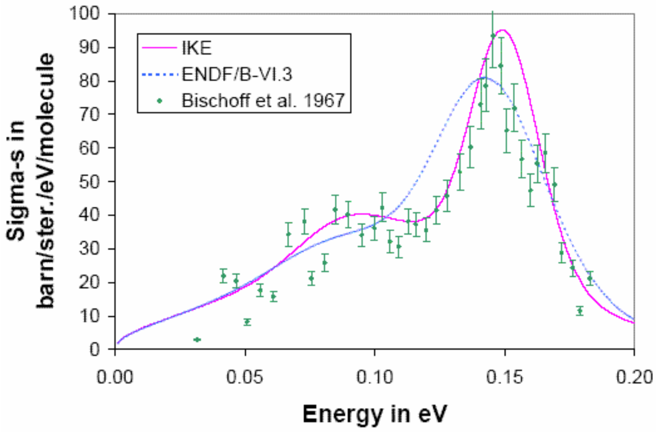
1. The precise value of the ^{1}H capture cross-section was the subject of some disagreement in the nuclear data community.
2. The low-energy scattering cross-section, as represented by the $S(\alpha,\beta,T)$ formalism in ENDF-formatted data libraries, was recently re-evaluated by M. Mattes and J. Keinert [72] at IKE.
3. Thermal reactor eigenvalues are very sensitive to ^{1}H-H_20 thermal scattering data.

[5] In addition to its dependence on the temperature through $\alpha(T)$ and $\beta(T)$, the scattering function has other temperature dependencies which complicate interpolation procedures.

A full description of the Mattes-Keinert evaluation is available in the INDC report [72]. Compared with previous ENDF and JEF evaluations, this new work proposes an improved modelling of water dynamics with a modified parameterisation of hindered rotation and translations as well as bending and stretching vibrations of the H_2O molecule. The new IKE model leads to a better prediction of the double-differential neutron scattering cross-section of water as shown in Figure 13.

Figure 13. Double-differential neutron scattering cross-section of water at room temperature computed with the ENDF/B-VI scattering data and the new IKE model, compared with experimental data of Bischoff, *et al*. [73]

Incident neutron energy = 154 meV, scattering angle $\theta = 60°$). The figure is taken from the INDC report [72].



More recent developments in this area are embodied in the new ENDF/B-VII.0 nuclear data library. The thermal capture cross-section of ^1H remains at 332.0 mb, although it is recognised that a fit to only the differential data gives 332.6 mb. Benchmark testing showed that the new Mattes-Keinert S(α,β,T) evaluation lowered thermal eigenvalues by the order of 100 pcm relative to ENDF/B-VI.8, due to small changes in the total cross-section. Modifications by MacFarlane [74] of the α and β grids reduced the impact of these changes to about 50 pcm, within the spread due to current code differences. The energies of the rotational modes were also slightly increased to bring the cross-section in the 50 meV region closer to the measured data. These changes increased the predicted k_{eff} by almost 200 cm in some cases.

Contributing to the remaining uncertainty, the total cross-section of bound hydrogen as a function of temperature is not specified in File 7 but must be reconstituted by a difficult integration in α,β space.

7. Conclusion

Good co-operation between reactor physicists and nuclear data evaluators was crucial in improving the prediction of thermal reactors and finding a credible solution to the k_{eff} underestimation problem. The status of new evaluations is as follows:

- The ^{238}U evaluation of resolved resonance parameters is completed. A preliminary version of this work was included in the JEFF-3.1 library released in 2005, and the final version was adopted in the β2 version of the future ENDF/B-VII library.
- The CEA/BRC evaluation of ^{238}U data above the resonance range was adopted in JEFF-3.1 and the new LANL work was included in ENDF/ B-VII.β2.
- With the help of recent ^{13}C(α,n) measurements, a new ^{16}O(n,α) evaluation performed at LANL, featuring a lower (n,α) cross-section, was proposed and adopted in ENDF/B-VII.β2.
- The new evaluation of ^{1}H-$H_2$0 thermal scattering data by Mattes, *et al.* was included in the JEFF-3.1 library. ENDF/B-VII.β2 includes a modified version of this evaluation proposed by MacFarlane.

The successive versions of new evaluations were continuously tested against k_{eff} measurements. The combination of the new inelastic data (LANL or BRC) with the new resonance-parameter set gives a satisfactory correction of the reactivity underestimation. Modifications to the ^{16}O and ^{1}H-$H_2$0 data have a slight influence on reactivity but contribute to the improvements. Most recent validation work of the new ENDF/BVII.β2 and JEFF-3.1 libraries confirmed the good prediction of uranium-fuelled thermal systems with the new data sets.

This work illustrated the importance of using large collections of benchmarks to assess the quality of the evaluated data.

8. Topics for future investigation

1. There should be a co-ordinated effort to compare the continuous-energy Monte Carlo codes. Despite the overall consistency observed between various codes using the same nuclear data, some differences in the calculated eigenvalues need to be understood. The existing comparison, often based on k_{eff}, should be extended to reaction rates in the thermal and epithermal energy range.

2. Recent studies suggest [75] that thermal lattices using mixed-oxide fuel are not well predicted with the newest nuclear-data libraries. This discrepancy requires further investigation and might be related to plutonium nuclear data. Accurate prediction of Doppler coefficient is still a challenging issue.

3. All the benchmarking presented in this report used fresh-fuel configurations. Modern nuclear data libraries tend to give consistent results in the prediction of k_{eff} at zero burn-up, but large differences are expected in depletion calculation at high burn-up. These differences are worth being understood. Clean integral experiments, easy to calculate and capable of measuring the k_{eff} versus burn-up, are still lacking.

4. Further integral tests are needed at high temperature to fully validate the new resonance parameters and thermal scattering data. It should be verified that the temperature reactivity coefficient is accurately predicted with the new files.

5. Several issues regarding the evaluation of the ^{238}U resonance range merit more extensive examination:

   - The evaluation of the ^{238}U p-wave resonance parameters and s-waves above several keV still needs some improvement. Statistical analysis of the ORNL/CEA resonance parameter shows that the traditional statistics deviate strongly from the GOE theory, indicating the presence of a significant proportion of missed and spurious resonances and of errors in spin determination.

   - Despite the low resolution of the available measurements, the energy range 10-20 keV was described by a set of resolved resonance parameters. As previously stated, the average cross-section deduced from resolved resonance parameters is lower by about 5% than that in the previous evaluations in ENDF/B-VI.8 and JEF-2.2, which used average resonance parameters. Further work should clarify this discrepancy.

   - The capture measurement performed by Moxon at Harwell [30] was not included in the ORNL/CEA fit because it was not available. The data were recently found and sent by Moxon to the NEA. Their analysis would be a valuable check of the parameters of the resonances below 100 eV.

   - Despite work at ORNL and CEA to identify the various sources of uncertainties, a full covariance matrix for ^{238}U cross-section is still not available and has been strongly requested by nuclear-data users.

6. As shown by Subgroup 9, the status of the ^{235}U prompt-neutron fission spectrum is still not satisfactory. Recent measurements are discrepant, and the most recent evaluation at LANL deteriorates the k_{eff} prediction of intermediate-spectra systems such as the highly enriched solutions described in the ICSBEP handbook.

7. New measurements of $^{16}O(n,\alpha)$ are in progress at IRMM [76] and should be compared with the new evaluation proposed by Page, *et al*. when the data are available.

8. In the discussion of solid-state effects, the modelling of the spectrum of elastically scattered neutrons in the ^{238}U resonances has been raised. The static model implemented in the current neutron-transport codes is crude. The need for a more rigorous crystal lattice formalism for resonant scattering, as in [77] and [78], in reactor calculations is still an open topic. The expected effect is an increase of the calculated ^{238}U capture rate due to upscattering of neutrons in resonances. A non-negligible impact on thermal-benchmark calculations might be expected as well.

9. Nubar (average number of prompt neutrons emitted in fission) is a very sensitive quantity for thermal benchmarks. At thermal energy, the prompt nubar of ^{235}U is accurately known but in the resonance range, differential experimental data [79,80] suggest significant fluctuations (of the order of 0.5%) which are currently not represented in the most recent nuclear data libraries. Both reliable measurements and modelling of the shape of nubar in the resonances are still lacking.

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