Status report of the WPEC/Subgroup-22

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1 Introduction

The subgroup-22 was formed 4 years ago to investigate nuclear data to improve the k_{eff} prediction of thermal benchmarks which are significantly underestimated by the most recent nuclear data libraries. This paper summarizes the evaluation work performed at several laboratories [Oak Ridge National Laboratory (ORNL), Los Alamos National Laboratory (LANL), Commissariat a l'énergie atomique de Bruyeres-Le-Chatel (CEA-BRC), International Atomic Energy Agency (IAEA)] as well as the integral tests (mainly at LANL, Knoll Atomic Power Laboratory (KAPL), Bettis Atomic Power Laboratory (BAPL), Nuclear Research and Consultancy Group NRG-Petten, CEA and IAEA) of the successive versions of the new evaluated files. The mandate of the subgroup-22 is ending this year and a final report is in preparation.

2 Summary of the past work (2001 - 2004)

The work has been summarized in a paper presented at the Nuclear Data Conference at Santa-Fe in october 2004 [1]. This section is a brief summary of this paper. The reactivity bias was observed for low-enriched thermal benchmarks after extensive integral tests of the ORNL ^{235}U evaluation of the resolved resonances [3] adopted in ENDF/B-VI.8, JEFF3.0 and JENDL3.3. It was demonstrated by the work of subgroup-18 [2] that the ORNL ^{235}U evaluation improves k_{eff} of highly-enriched uranium (HEU) critical systems and corrects the longstanding underestimation of ^{236}U build-up in pressurized water reactors (PWR). However, studies by Kahler et al. [4], Weinman et al. [5] and Van Der Marck and Hogenbirk [6] involving low enriched thermal benchmarks mainly from the ICSBEP (International Criticality Safety Benchmark Experiment Project) and CSEWG (Cross-Section Evaluation Working Group) benchmarks book confirmed a systematic eigenvalue under-estimation of about -500 pcm with the newest nuclear data libraries.

^{238}U integral trends in thermal and epithermal range The resonance parameters of ^{238}U are the same in ENDF/B-VI.8, JEFF3.0, and JENDL3.3, and are the result of an evaluation work performed by Moxon et al. [7]. Integral trends on ^{238}U cross-section were studied by different methods :

- k_{eff} bias versus ^{238}U capture fraction (Kahler [4] and Weinman [5]);

- interpretation of ^{238}U spectral indices : ρ^{28}, $C^{*} = \sigma_c^{U238}/\sigma_f^{U235}$, C^{U238}/F^{tot} performed in the EOLE facility in France [8], in the IPEN Brazilian mock-up [9] and in the TRX and the DIMPLE reactor [10];
- analyses of Hellstrand experimental correlations [11] (measurements of effective capture resonance integral [12], [13], [14]);
- post-irradiation experiments (^{239}Pu production versus burn-up) [15].

Those studies did not demonstrate significant discrepancies with the ^{238}U evaluation of Moxon: the calculated spectral indices, ^{239}Pu build-up, or effective resonance integral values, are generally within the uncertainty of the integral measurements, demonstrating the quality of the Moxon resonance parameters set. Nevertheless, these results suggest a small decrease of the ^{238}U effective capture resonance integral by about 0.5% to 1.0%, which is considered to be within the experimental uncertainty of both present day integral and differential measurements

Evaluation of ^{238}U thermal capture cross-section value Different recommended values for the ^{238}U thermal capture cross-section can be found: $\sigma_0 = 2.708\ b$ from the CSEWG recommendation [16], $\sigma_0 = 2.718\ b$ with the positive and negative-resonance parameters of Moxon, and 2.680 ± 0.019 b from the latest Mughabghab work [17]. The ^{238}U(n,γ) thermal cross-section was reviewed by A. Trkov et al. [18]. Some of the activation data selected for the evaluation are based on the measurements of γ activity from the β decay of ^{239}Np. Because the derived cross-section value is strongly correlated to the knowledge of γ-ray emission probability, a review of existing measurements of γ line production data was also performed. In addition, the measurements carried out in Budapest and published recently [19] were reanalyzed in depth to get new γ-ray experimental data. The final least squares fit, performed with the ZOTT99 code, gives a final value of $\sigma_0 = 2.683 \pm 0.012\ b$.

Evaluation of ^{238}U resolved resonance range A new evaluation of resonance parameters was undertaken at ORNL. Several successive versions were distributed to the working group for benchmarking and the latest version called ORNL4 was presented at the 2004 Santa-Fe conference [20]. Fits of selected differential measurements were performed with the Reich-Moore formalism implemented in SAMMY. The Harvey et al. high resolution transmission measurements [21] performed at the Oak Ridge Electron Linear Accelerator (ORELA) in 1988 were used for the first time in the ^{238}U evaluation extending the resolved range from 10 to 20 keV. The capture data of Macklin [22] (ORELA) from 250 eV to several hundred keV were completely analyzed.

The energy range below 1 keV, crucial for the calculation of thermal reactors was carefully investigated and is summarized here. The thermal capture value was adjusted to $\sigma_0 = 2.683\ b$, following the previous recommendations. The shape of the capture cross section in the thermal range was checked against the capture measurements of Corvi et al. [23] performed at GELINA. For the large s-wave resonances at 6.7, 20.8 and 36.6 eV, the seven transmission spectra of Olsen [28] were fitted using the four transmission measurements performed at room temperature at GELINA by Meister et al. [25] and the capture measurements of de Saussure et al. [24]. As discussed in another paper [26] presented at ND2004, the Crystal Lattice Model (CLM [29]) of SAMMY was used to describe the shape of the 6.7 eV resonance. Resonance parameters values below 100 eV are displayed in Table 1 when the radiation widths are fitted and when kept to the

Moxon values. Extracted Γ_γ are slightly higher than those of Moxon. For ORNL4, the Γ_γ of Moxon was adopted and fixed below 100 eV and the neutron widths were fitted (see last column of Table 1). The resulted resonance parameters were found to give better results on thermal benchmarks. Further work eventually provided a better justification of the choice of these parameters as explained in the next section.

Energy	Γ_γ meV present work	Γ_n meV present work	Γ_γ meV ENDF/B-VI	Γ_n meV ENDF/B-VI	Γ_n meV present work Γ_γ from ENDF/B-VI
	R' = 9.45 fm		R' = 9.42 fm		R' = 9.45 fm
6.674	23.01 ± 0.02	1.475 ± 0.001	23.00	1.493	1.476 ± 0.001
20.871	23.12 ± 0.03	10.04 ± 0.01	22.91	10.26	10.07 ± 0.01
36.682	23.41 ± 0.04	33.43 ± 0.02	22.89	34.13	33.55 ± 0.02
66.031	23.64 ± 0.10	24.17 ± 0.04	23.36	24.60	24.23 ± 0.03
80.747	23.31 ± 0.41	1.877 ± 0.01	23.00	1.865	1.877 ± 0.01
102.56	24.53 ± 0.14	70.62 ± 0.08	23.40	71.70	71.03 ± 0.08

Table 1: Resonance parameters of the ^{238}U s-wave resonances when the radiation widths are fitted (left) and when kept to the ENDF/B-VI values (Moxon et al. [7]). The small uncertainty values quoted in this table takes into account only the statistical uncertainty of the measurements. The actual values accounting for systematical uncertainties are much larger.

The main effect of this new resonance parameters is a slight decrease of the effective capture resonance integral by about 0.4% mainly due to smaller neutron widths of the lowest s-wave resonances. A more detailed description of the evaluation especially above 1 keV can be found in the Santa Fe paper.

New evaluation of ^{238}U inelastic scattering data Over the past 20 years, a large effort has been devoted to the improvement of the modeling of the ^{238}U cross-section above the unresolved range. In 1989, in the framework of the subgroup-4 [27], a set of measurements on ^{238}U(n,n') were performed to solve discrepancies and reduce uncertainties in the previous data. Experimental neutron spectrum, partial cross-section measurements listed in [27] gave valuable information on optical model parameters. In the meantime, coupled channel and statistical models have been improved to predict the ^{238}U inelastic cross-section. As a result of subgroup-4 efforts, improved evaluations of ^{238}U have been released by Maslov et al. [30] and Kawano et al. [31]. Recently, two independent evaluations by the Los Alamos National Laboratory and Bruyeres Le Chatel (BRC) groups were undertaken and successive releases were distributed to the subgroup-22 for discussion and testing purposes. This work was presented at the Santa Fe conference (Young et al. [33], Lopez-jimenez et al. [34]) Compared with older ENDF/B-VI.8 and JEF2.2 evaluations, performed before the formation of subgroup-4, the comparison with experimental data, in particular, neutron emission spectra [32] (inelastically scattered neutron + fission) at different incident energies, is much improved by these new files. The common feature of the new evaluations is a much softer inelastic secondary neutron spectrum compared with the previous one adopted in ENDF/B-VI.8 or JEF2.2. The influence of these new data on ICSBEP thermal benchmarks was found to partially correct the reactivity bias by reducing the neutron leakage rate.

Integral testing The different versions of evaluations in the resolved range and above the unresolved range have been continuously tested against k_{eff} measurements. Some inter-comparisons have demonstrated the overall consistency of the calculated eigenvalues between Monte Carlo codes (MCNP - RACER - RCP - TRIPOLI4) using the same nuclear data libraries. Some differences were noticed (up to 150 pcm for some leu-Comp-Therm configurations between TRIPOLI4 and MCNP) and, so far, could not be explained by the statistical uncertainty inherent in Monte Carlo calculations. Investigation of these differences would require a more rigorous comparison (neutron balance, reaction rates and so on) to identify whether it comes from differences in benchmark modeling, processing methodology, transport methods or assessment of statistical uncertainty in Monte-Carlo codes.

The differents versions of the ORNL resolved-range evaluation and the fast range data from LANL and BRC were merged in two complete ^{238}U test files (ORNL + LANL) and (ORNL + BRC). Integral testing of these files has demonstrated the improvement of reactivity prediction for Low-enriched thermal lattices of ICSBEP [36], [35]. A paper presented by Mac Farlane [37] at Santa Fe gives a summary of the performance of the new files using MCNP5. It was also noticed that the present ^{238}U data preserves a good C/E agreement (with JEFF3.0 and ENDF/B-VI.8) for other kind of uranium systems such as Leu-Sol-Therm, Heu-Sol-Therm.

3 Recent work April 2004 - April 2005

Since the last WPEC Meeting in 2004, the following progress have been made:

- Most of the benchmarking tests have been previously carried out with the version 3 of the ORNL evaluation. After the release of the Version 4 at the Santa Fe Conference in october 2004, several checks have been done (Sublet [42], MacFarlane [43]) to confirm that the latest evaluation still preserves the performance of ORNL3. It is worth mentioning that the ORNL4 resonance-parameter set associated with the fast range data from BRC was adopted in the JEFF3.1 starter file.

- Evaluation work at ORNL is still in progress for a better justification of the resonance parameters at low energy (value of Γ_γ) and to improve the quality of the fit up to 20 keV. A revision of the external levels as well as the effective radius ($R = 9.48\ fm$) led to a better agreement with the average experimental transmissions of Harvey et al. and Olsen et al. (averaged over 1 keV interval). Fits have been performed again especially at low energy and the extracted radiative widths are now very close to Moxon's value, neutron widths still being lower. The value of I_{eff} is still the same as ORNL4, giving the same improvement in k_{eff} prediction. Other less important topics have been investigated such as the evaluation of the neutron coherent length (linked to the thermal scattering cross section), estimate of the direct capture at thermal and keV energies (neglected in the present work), the study of "classe II" resonances featuring low Γ_γ. A new file ORNL5 should be made available in the near future. Statistical tests in the framework of circular orthogonal ensemble (COE) developed by Dyson and coworkers are in progress at ORNL to check the overall quality of the ^{238}U resonance set (comparison with Wigner level spacing and reduced neutron widths Porter-Thomas distribution, Δ_3 statistics, F-Dyson statistic, correlation coefficient between nearest neighbor level spacing). This analysis provides a new evaluation of the strength function and the level average spacing.

- In the framework of the evaluation of standard cross section, Carlson [38] has recently proposed a new evaluation of the ^{238}U capture up to 2 MeV. ^{238}U capture is not considered as a standard but is a by-product of the evaluation work. This new analysis has justified a revision of the LANL evaluation above the unresolved range. The new file should be available soon.

- A new evaluation of the unresolved resonance parameters (from 20 keV to 150 keV) has started at ORNL using the latest high resolution transmission experiments from Harvey et al. [21] and Macklin et al. [22]. However, this new work should not have a significant impact on thermal reactors eigenvalues.

- Using pincell benchmarks, significant differences in temperature effects were pointed out by Huriah between preliminary ENDF/B-VII and current ENDF/B-VI libraries. This problem is being studied at JAERI(Dr Wu) using the KRITZ2 experimental cold and hot configurations and differences in the prediction of isothermal reactivity coefficient is indeed observed. First analyses suggest that the new ^{238}U files is not responsible for these differences. Other nuclear data such as ^{235}U or water cross sections could explain the observations.

4 Main conclusions

The latest release of ^{238}U evaluation of resonance parameters (called ORNL4), presented at the Santa-Fe conference by the ORNL group adopts the thermal capture cross section recommended by Trkov and proposes a slightly lower capture resonance integral (-0.4% for a 50 b dilution) that improves the prediction of k_{eff} for thermal systems. Minor revisions are in progress before the release of the final version (ORNL5).

The new evaluations of ^{238}U inelastic scattering data from both LANL and BRC also contribute to the correction of the under-estimation. Finalized version of the LANL evaluation is expected soon. The association of the new resonance parameters and inelastic data gives a satisfactory solution of the k_{eff} under-estimation problem.

Although, the working group is still dealing with preliminary versions of evaluations, the final versions of the ^{238}U files, to be released soon, are not expected to change these conclusions.

5 Topics for future investigation

Many topics regarding the improvement of nuclear data impacting thermal benchmarks have been mentioned in the *ueval@nea.fr* discussions. The final report will provide a list of topics that would require further work. It is worth mentioning the following points which have not been studied in detail and need a closer look.

- A rigorous inter-comparison of Monte Carlo Codes would help to understand the differences observed in k_{eff} prediction among the various codes such as MCNP, TRIPOLI, RACER, RCP. Such comparisons using the same nuclear data have not been performed rigorously within the working group and should deal not only with eigenvalues but also neutron balance and reaction rates.

- Difference in temperature effects observed using preliminary ENDF/B-VII files merits further investigation.

- Large differences between libraries are observed for the O16 (n, α) cross-section above 3 MeV, JENDL3.2 O16 (n, α) being significantly lower than in ENDF/B-VI.8 and JEF2.2. In the analysis of Hale et al. [39] and Sayer et al. [40] $\sigma_{n,\alpha}$ cross-sections are deduced by reciprocity from $C13(\alpha, n)$ measurements. In the energy range 3-6 MeV, differences up to 50% are pointed out between the various $C13(\alpha, n)$ experimental data. A new measurement is recommended to remove these discrepancies. The use of JENDL3.2 instead of ENDF/B-VI.8 or JEF2.2 produces a slight increase of $\approx$ 50 pcm in typical thermal benchmark.

- Subgroup-9 devoted to neutron fission spectrum pointed out large discrepancies in the peak and in the tail region between the two most recent measurements of U235 spectrum for thermal neutron. The latest evaluation proposed by David Madland is still preliminary but the current uncertainty on the shape of U235 thermal spectrum was found to have a significant impact on k_{eff} of HEU and LEU systems. Despite the work done at Los Alamos to solve the discrepancy and improve theoretical modeling, a highly accurate measurement of the U235 thermal fission spectrum is needed.

- New spectral ^{238}U indices experiments are planned in the French EOLE facility and the Brazilian reactor IPEN and will provide further checks of ^{238}U resonance parameters. More extensive analysis of ^{239}Pu production in PWR is also recommended.

- New analyses of ^{238}U unresolved resonance parameters have been reported in the recent year. Even though the effect of these new average parameters on thermal reactor is expected to be small, integral testing using thick samples transmission experiments and/ot k_{eff} of fast reactor would be useful before inclusion in libraries.

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