Summary report of the WPEC/Sub-Group-22 Nuclear data for improved LEU-LWR Reactivity predictions

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Abstract

This report is a summary of the WPEC/Sub-group-22 activities and the related "ueval" website discussions. The sub-group was set-up to deal with the "LEU-LWR reactivity under-estimation problem" (**L**ow **E**nriched **U**ranium fuel, **L**ight **W**ater **R**eactor). The main task of the working group is to confirm the under-prediction and investigate the main nuclear data impacting the calculation of thermal systems eigenvalue. A close association between nuclear data evaluators and reactor physicists is the keypoint to solve the problem.

1 Objectives of the WPEC/Sub-Group-22

This new sub-group was created 6 months ago at the WPEC Meeting held at GEEL 23-24 May 2002. The main objective is to address the so called "reactivity under-prediction problem" for thermal LWR systems. Arnaud Courcelle from CEA-Cadarache (arnaud.courcelle@cea.fr) is the co-ordinator and Richard McKnight from Argonne (rdmcknight@anl.gov) is the monitor. The sub-group proposal is available at the WPEC web page :

http://www.nea.fr/html/science/wpec/index.html.

The short term goals can be summarised as follow :

- analyses of integral trends to confirm the LEU-LWR reactivity bias with the most recent nuclear data libraries ;
- investigation of the discrepancy between the U238 capture rate integral measurements and the current evaluation ;
- investigation, if needed, of other nuclear data (H2O, O16, U235, U238) impacting thermal reactor eigenvalues ;

The main aim is to provide suitable recommendations to solve the problem. The communication within the group is mainly assured through the NEA mailing list called ueval *http://www.nea.fr/lists/ueval.html.* The present paper is a summary of the discussion with the main scientific contributions of : Yung-An CHAO (Westinghouse), Arnaud COURCELLE (CEA), Christopher DEAN (Serco Assurance), Alfred HOGENBIRK (NRG), Harish C. HURIA (Westinghouse), Albert C. KHALER (Bettis Atomic Power Lab), Cecil R. LUBITZ (Knolls Atomic Power Lab), Michael C. MOXON, Alain SANTAMARINA (CEA), Andrej TRKOV (AIEA) and James P. WEINMAN (Knolls Atomic Power Lab). Others have also contributed, the complete list "ueval" subscribers is available in the ueval website.

2 Analysis of integral trends

LEU-LWR eigenvalue calculation The reactivity bias for thermal critical system was observed after extensive integral tests of the ORNL U235 evaluation in the resolved range [1] adopted in the major nuclear data libraries. Several years of investigation has demonstrated that this new evaluation significantly improves integral calculations (highly enriched systems reactivity calculations, U236 build-up prediction in PWR) and is probably not the source of the under-estimation. Before the set-up of the sub-group, several Continuous Energy Monte-Carlo (CEMC) studies had raised the problem [3], [4], [5], [6], [7]. According to these criticality studies involving thermal benchmarks mainly from the ICSBEP handbook and CSEWG benchmarks book, a systematic eigenvalue under-estimation ranging from -600 to -200 pcm is deduced with most recent nuclear data library using U235 resolved range from ORNL and U238 resolved range from Moxon et al. [2]. Work is under progress to confirm these trends with a more extended integral database and the newly released library (ENDFB6.8, JEFF3.0, JENDL3.3). **One important task is to check the consistency among the various Monte-Carlo codes so that the reactivity bias could be reliably linked to basic nuclear data.** Even if a greater place is given to Monte-Carlo approach, deterministic caclulations which are valuable for trend and sensitivity analysis, are not excluded. For instance, in the framework of the WIMS-D Library Update Project (WLUP), A. TrkoV uses a large set which includes about 200 benchmarks of different type, enrichment and spectrum hardness (see NEARCP-U-190 report and *http://www-nds.iaea.org/wimsd/*).

Hellstrand correlation : measurements of U238 effective capture resonance integral Based on bibliographic information (see for exemple [8] and [9]), discussions has highlighted two different approaches to analyse Hellstrand's correlations (measurements of effective U238 capture resonance integral as a function of isolated rod geometry) with Monte-Carlo code : the first consists of interpreting in detail one particular experiments (requiring to know the actual geometry of the experimental region and the detailed procedure to deduce the effective resonance integral). The second way is to calculate the effective integral on a simple geometry representing the isolated rod with a 1/E neutron source . This latter approach is valid under various assumptions (no Dancoff, pure scattering moderator, experimental results corrected from the deviations of 1/E neutron spectum). However, given the 3.5% uncertainty, quoted by Hellstrand, these experiments should be only considered as a supplementary check to test the current U238 evaluation.

Measurements and analysis of U238 spectral index Spectral indices in selected proprietary French experiments performed in the EOLE facility (MISTRAL and ERASME configurations) were analysed [10] with the TRIPOLI4 code (cell calculation corrected with deterministic calculations to take into account neutron leakage). From this study, an average overestimation of the U238 capture rate equal to $+1.5\% \pm 1.0\%$ (1σ) is calculated. A recent study [11] presented at the PHYSOR 2002 conference reports new measurements of U238 spectral indices by two different techniques (direct gamma spectrometry of the fuel pin and measurements with uranium foils) in the IPEN/MB01 reactor. The measurements were carefully analysed by the authors with the Continuous Energy Monte-Carlo code MCNP4B (ENDF/BVI.5 library) and their results also pointed out an over-estimation of the U238 capture in reactor (same magnitude as the EOLE experiments). **A review and analysis of the major U238 spectral index (such as those performed in TRX or BAPL critical facilities [12]) is still desirable to draw more accurate trends**.

3 U238 evaluation in the thermal and resolved range

In this section, a brief summary of the *ueval* discussions related to the current U238 evaluation is presented.

U238 Thermal capture value An important task for the subgroup is still to recommend a thermal value for the capture cross-section and find out why the Mughabghab and the CSEWG standard committee do not recommend the same value (2.68/2.708b).

Solid State effect The study [13] has demonstrated that the use of the Free Gas Model (with an effective temperature) in the evaluation of the first two larges resonances of U238 lead to biased resonance parameters (in UO2 and U metal sample). Nancy Larson has implemented the crystalline model (based on the DOPUSH code [13]) in the new version of SAMMY. The implementation is being tested against U238 transmisson measurements performed at GEEL in 1994 (UO2 and U metal sample at low and room temperature) [14]. It is also expected to compare the results given by SAMMY and REFIT to check the implementation of the crystalline model in the two codes and confirm the conclusions of [13].

Reich-Moore approximation : Capture interference effect In the 1975 U238 Seminar [15], Bob Chrien pointed out that the Reich-Moore approximation is violated for U238. In this R-matrix approximation [16], off-diagonal contribution from photon channels to the level matrix are neglected because of a large number of exit channels for photon radiation with decay amplitude of comparable magnitude and random signs. However, nuclear spectroscopic studies of the U239 compound nucleus have demonstrated the existence of a preferential decay to a single low-lying level [17]. This may change the shape of the 6.67 eV resonance in the wings introducing a significant assymetry. In order to display "non Reich-Moore" interference effects, M. Moxon has performed REFIT calculations in which a fraction of the radiation width was transferred to the unused fission channel. Various assumption have been tested about the signs of the radiative width amplitudes and the part transferred into the "fission" channel.

He concluded from these calculations "that interference effects in the capture reaction are not very large and might account for some of the discrepancy, especially for heavily shielded samples, where a lot of capture is taking place in the region between the resonances and if there are some negative interference effects.". Work is in progress to evaluate the effect on thermal reactor.

Adjusted cross-section Cecil Lubitz proposed an adjustment of the U238 resonance parameters. The adjustment is based on the average radiation width value deduced from the analysis of unresolved range (10 keV - 300 keV) by Fritz Frohner [18] : $\Gamma_\gamma = 22.65\ meV$. In the resolved range (up to 10 keV), the average radiation width value from the Moxon et al. analyses is $\Gamma_\gamma = 22.96\ meV$. In the present adjustment, all s-wave radiation widths were reduced by 1.35% which is the ratio of the average Γ_γ in the urr to that in the rrr. It was chosen to adjust slighly Γ_n values to keep in the adjusted total cross-section the doppler-broadened peak height of each resonance. The resonance adjustment procedure is similar to the one used in the study [19] of the U235 epithermal capture cross-section. Furthermore, the radiation widths of the negative-energy resonances were increased to set the 2200 m/s capture value to 2.708 barns (CSEWG standards value). The ENDF formatted file ditributed to ueval is not considered as a recommended data set and was created for sensitivity studies only.

Compared with the original evaluation, the effect of this adjustment is to reduce the thermal capture value by 0.4% and the effective (diluted) capture integral by 0.7%. The new U238 file was tested by Jim Weinman using Continuous Energy Monte Carlo calculations with the Valduc experiments LEU-COMP-THERM-007 and LEU-COMP-THERM-0039. From these calculations, it is concluded that the proposed changes in U238 s-wave resonance data cause an increase in predicted reactivity (from 50 to 150 pcm in average with a Monte-Carlo statistical uncertainty of 40 pcm (1σ)). A TrkoV evaluated the effect with determistic WIMS calculations on a large set of critical benchmarks. A reactivity increase in the benchmarks containing U238 is also demonstrated (from 100 to 200 pcm).

U238 resonance parameters evaluation Mention should be made of the work planned on U238 evaluation at the Oak Ridge National Laboratory [22]. This work includes the extension of the resolved resonance range up to 15 keV. It is also planned to perform the analysis of the resonances at low energy by using all the available experimental data with the new Doppler broadening possibility of SAMMY.

4 Other nuclear data

The integral trends has focused the discussion on the U238 resonance parameters, however LEU-LWR reactivity calculations are sensitive to several isotopes (mainly U235, U238, H2O, O16) and it is not excluded that the current eigenvalue under-estimation may come from other nuclear data. In the early discussions, several issues summarised here have been discussed :

O16 : It has been noticed that there are large differences between the evaluations for the O16 (n,α) cross-section above 3 MeV. JENDL3.2 O16 (n,α) is significantly lower than the ENDFB6 values. The reduction of the (n,α) cross-section from JEF2.2-ENDFB6 to JENDL3.2 would increase the LWR-UOX reactivity by about 100 pcm. In the various recent evaluations [20], [21] $\sigma_{n,\alpha}$ cross-sections are generally deduced by reciprocity from $C13(\alpha,n)$ measurements. It is worth noting that, in the low energy range 3-6 MeV, large differences (10% to 50%) are observed between measurements [21]. Consequently, the absolute uncertainty of the current evaluations is probably large and there is a need for new O16(n,α) measurements in the 3-6 MeV. However, the most recent O16 evaluations have independantly recommended high (n,α) value close to the ENDFB6 evaluation.

U238 inelastic data : It has been pointed out in the early ueval discussion that changes to the U-238 inelastic scattering and elastic angular distribution data could affect the caculation of thermal reactor eigenvalue. J. Weinman calculated with monte-carlo code the most sensitive of the benchmarks with substituting U238 inelastic files from JENDL 3.2 into the ENDF6.5 evaluation. A surprisingly large reactivity effect is observed : the average eigenvalue for the selected thermal benchmark increased by $\sim$ 250 pcm. A study performed by A. TrkoV with WIMS has led to similar conclusions with the JEF2.2 nuclear data : the replacement of the JEF2.2 elastic angular distributions and inelastic data results in an increase of the multiplication factor for well thermalised lattices. The average increase for the thermal lattices amounts to 160 pcm in the case of JENDL-3.2 data and 270 pcm in the case of CENDL-2.1 data. However, the cause of the improved reactivity performance of the Valduc benchmarks with the use of the JENDL3.2 U238 is mainly from a reduction of the neutron migration area. Therefore, it is concluded that the changes of U238 inelastic data will only affect small size configurations such as the VALDUC experiments for instance which have high neutron leakage.

5 conclusion

This document is an attempt to summarise the most important contributions posted in the *ueval* website. From this work, the following conclusions can be drawn :

- Numerous studies based on Monte-Carlo calculations have provided firm evidence for LEU-LWR reactivity underestimation with the most recent libraries (JEFF3.0, JENDL3.3 and ENDFB6.8). The magnitude of this systematic underestimation (ranging from about -200 pcm to -600 pcm) depends on the nuclear data library and work is in progress to derive reliable trends (reactivity bias as a function of spectrum hardness for instance)

- Based on integral measurements of U238 spectral indices, several analyses have pointed out an overestimation of the U238 reaction rate with the current evaluation. In the framework of the working group, **it is a priority to extend the analysis to accurately determine the magnitude of this integral overestimation**.

- From the previous conclusion, the working group is investigating various topics concerning the current U238 evaluation in the thermal and resonance range : thermal capture value, solid state effect, sensitivity studies, re-evaluation, in order to find explanations for the differential/integral discrepancy.

- Up to now, no simple solution has been found to solve the problem, it is not excluded that the solution is a collection of small changes not only on U238 capture cross-section but also on other nuclear data (U238 inelastic data, U235, O16, H2O).

It is believed that the problem can be solved only through a close collaboration between cross-section evaluators and reactor physicists. However, given the limited number of volounteers contributing the sub-group-22, **additional help from both evaluators and reactor physicists is strongly needed**.

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