Summary Record of the 3rd Meeting of WPEC Subgroup 39 on

Methods and approaches to provide feedback from nuclear and covariance data adjustment for improvement of nuclear data files

NEA, Issy-les-Moulineaux, France

27-28 November 2014

The subgroup co-ordinators, **M. Salvatores** and **G. Palmiotti**, welcomed the participants to the meeting (see list in Appendix 1). **O. Cabellos** is presented as the new WPEC secretary. The proposed agenda was adopted with minor changes (see Appendix 2).

M. Salvatores reminded the participants of the subgroup objectives and reviewed the actions agreed at the previous meeting. These actions will be discussed and updated during the meeting (see section 7). It was agreed to report the results of this meeting to all participants of the SG39 who have not attended this time.

1. Sensitivity Methods

M. Aufiero presented the developments/implementation of a collision history-based approach to GPT calculations in SERPENT code. This implementation permits to perform perturbation/sensitivity calculation (e.g. keff); also it is applied to reaction rates. Examples in Flattop-Pu, UAM TMI-1 PWR pin-cell and Jezebel were presented. The method can be extended to scattering distribution sensitivities, although results for sensitivities to scattering distributions have not been fully tested/verified yet. **M. Aufiero** acknowledges VTT developer team who are delivering a new version of SERPENT code with the sensitivity/uncertainty capability.

I. Kodeli presented a comparison of deterministic (XSUSA/TWODANT, ERANOS/PARIS, TSUNAMI-3D, SUSD3D/PARTISN/TWODANT/THREEDANT) and Monte Carlo (SERPENT2, MCNP6 is ongoing) sensitivity analysis of SNEAK-7A and FLATTOP-Pu Benchmarks. For SNEAK7A&7B, calculations of the keff and βeff to the nuclear cross-sections were shown. Good consistency was observed between the sensitivities, both integral values and sensitivity profiles. Discrepancies with U^{238} (n, elastic) using TSUNAMI were identified. It was concluded that βeff is also of interest for the SG39, since sensitivities are quite different from those of keff, the term of delayed neutron emission having an important effect.

2. Integral Experiments

M. Hursin reviewed the PROTEUS FDWR-II (HCLWR) program experiments for Core 7, 8 & 9 with modern modelling tools (MCNP6 & SERPENT-v2 (2.1.15)). Consistent sensitivity information was generated with SERPENT-2 and MCNP6, where sensitivity profiles are different to Flattop. Regarding with the issue of dissemination of information, the data itself may or may not go for free. At this point, it was mentioned that only C/E (with associated uncertainties) and sensitivity profiles according to SG33 format would be required, minimizing the cost of providing the full set of data and avoiding to provide experimental values.

M. Salvatores presented "PROTEUS Experiments, HCLWR configurations" to be considered in the priority list for sensitivity analysis.

I. Kodeli, presented the status of SINBAD Benchmark Database. Ivo reported some completed quality evaluations done in 2012-14, not yet in SINBAD, but having great interest in SG39: JANUS and ASPIS Experiments. In addition, SINBAD Benchmarks using TOF technique were also reported, and more detailed information is given for the FNS-Liquid O TOF Benchmark. The analysis is performed with MCNP-6 Monte Carlo in energy and time domain (ENDF/B-VII.1, and SG40/CIELO files provided by L. Leal are used) obtaining little difference of calculated spectra. It can be concluded that FNS Liquid Oxygen benchmark is suitable for validation of O cross-sections including angular distributions of secondary particles.

D. Da Cruz presented the STEK experiments to be used to improve nuclear data evaluation for fission products. STEK experiment is modelled with MCNPX. Reactivity worth caused by Carbon, Indium, Europium and Tc^{99} samples were simulated for 5 different STEK configurations. These results could give important information to the evaluators to try to improve the nuclear data for these elements (other elements e.g. U235, B^{10}, Fe^{56},…). On-going activities: the development of a new STEK model for DRAGON code. At this point, it was mentioned that, in this case also, only C/E and sensitivity profiles are needed for contributing in SG39. It was asked to verify if the reactivities of isotopes other than fission products (e.g. U-235, U-238, Fe etc.) were available in the different configurations.

M. Salvatores presented some detailed information on STEK and SEG experiments. The information is available in several documents, in particular at CEA-Cadarache (JEFF/DOC-861) and at former JNC (TN9400 2001-043). Both STEK and SEG experiments are very interesting from the physics point of view: i) systematically variable neutron spectrum hardness changing nuclear configurations (STEK), ii) ad-hoc tailored adjoint flux shapes to reduce/amplify reactivity effects due to scattering (SEG), where the shape of the adjoint fluxes in these experiments can be used to estimate the importance of capture (flat adjoint) or elastic (sharp adjoint) reactions. It was also noticed that these experiments are not easy to analyse (coupling effects thermal-fast, self-shielding effects) and experimental uncertainties sometimes are significant. It was concluded that both types of experiments were still very interesting for the SG39 objective to introduce experiments in order to separate specific isotope and reaction effects. However, in the case of SEG, it would be useful to make some new exploratory studies to understand the possibility for their utilisation. INL volunteers to do that.

T. Ivanova presented IPPE transmission experiments: Fe (FUND-IPPE-VdG-MULT-TRANS-001), 238U (FUND-JINR/E-MULT-TRANS-001) in the ICSBEP-Vol. IX (Fundamental Physics Measurements Supporting Nuclear Criticality Safety). It was mentioned that detailed information on uncertainties are reported in these Benchmarks. For U^{238}, the explicit product of the experiments was the measurement of the energy-dependent self-shielded total and fission cross sections. Self-shielding was varied systematically through the use of samples of different thicknesses. It was remarked that a good agreement on C/E is obtained using 28 groups- ABBN93 library. Other IPPE, LLNL, and NIST experiments were also mentioned. Other interesting issue is how to calculate sensitivities in these experiments.

G. Palmiotti presented the talk given by Y. Danon in the 2014 CSEWG/CIELO meeting. Activities on nuclear data measurements at RPI were summarized: 1) U^{235} fission and capture up to 3keV, 2)Fe^{56} –high resolution transmission between 0.5 to 20 MeV, 3) neutron scattering 0.5-20 MeV for U^{238} and Fe^{56}. Simulations of the experimental ^{nat}Fe irradiation with MCNP and JENDL4 had a good overall agreement. This measurements and MCNP simulations can be used as benchmark for cross section and angular distribution evaluations. It was noted and to be considered by SG39 that there is a risk taking into account twice the adjustment in differential and integral evaluation.

G. Palmiotti presented some activities under way at the EG-IEMAM (Expert Group on Integral Experiments for Minor Actinide Management). Focus is put on isotopes of interest such as: Np^{237}, $Am^{241,242m,243}$, $Cm^{243,245}$. Experiments based on different techniques (irradiation, reactivity oscillation,…) would be valuable for improving the minor actinide cross sections.

S. Pelloni presented the work done at PSI on adjustment studies accounting for nonlinearity. The work is focused on ERANOS and the associated data libraries which form a reference deterministic tool for fast spectrum system calculations. It accounts for nonlinearity by means of iterative procedure: Repeated calculation of sensitivity coefficients with adjusted cross-sections; multiple, stepwise adjustment. See more details in: *Annals of Nuclear Energy, **72**, p. 373-390 (October 2014).* Using this method, an improvement by accounting for nonlinearity is found. However, stronger adjustments are required. There are still some issues to be explained: 1) large adjustment are required (e.g. inelastic), and 2) it has been found some inconsistencies of adjusted cross-section when different prior data bases are used. It was noted that this methodology should assess the correlations between different isotopes.

3. Am-241 and fission product issues

A. Barnes (by telephone-conference) presented the need to establish a reliable safe mass limits for Am^{241} to be used by EU in space application. The term associated for error due to program and nuclear data (E_{PD}) is unknown (lack of critical experiments, uncertainty in nuclear data, variations in nuclear data processing, computational tools,…). A summary of the forward plan presented is: 1) understand, attribute and quantify the current nuclear data uncertainties, 2) identify potential benchmark experiments, 3) improvements/adjustment to nuclear data, 4) specify theoretical benchmarks, 5) propose suitable integral experiment programme, 6) propose a nuclear data set suitable for use in a criticality safety case, quantifying its uncertainties. Some activities are related with NEA activities: SG39, SG41, WPCNS, ICSBEP,…

G. Palmiotti, all , discussion on the main isotopes to be investigated by SG39. It was agree that the five isotopes of interest are: Na^{23}, Fe^{56}, $U^{235,238}$ and Pu^{239}. Other isotopes to be considered in SG39 are: $Am^{241,242m,243}$, Np^{237}, $Cm^{243,245}$, …, O^{16}, …,Fission products (Pd^{105},…), …

4. Covariance data

K. Yokoyama recalled the work "Covariance Data of JENDL-4.0 and ENDF/B-VII.1 by M. Ishikawa". In that study, some important issues for SG39 were discussed: 1) For ^{239}Pu capture, reason for the discontinuity of the uncertainty at 2.5Kev in ENDF/B-VII.1. 2) For ^{235}U fission, reason of 5% uncertainty in the range of 500eV~9keV, and sharp peak around 2keV (NJOY problem?). 3) For ^{235}U capture, better understanding of the uncertainty both in JENDL-4.0 and ENDF/B-VII.1. 4) For U^{238}, in the unresolved region of 20~100keV, the STD of JENDL-4.0 is significantly larger than that of ENDF-7.1, and vice versa in 100~150keV. 5) For U^{238} inelastic and elastic, cross-sections of JENDL-4.0 and ENDF-7.1 seem quite similar, but the STD values and the shapes are completely different. 6) For Fe^{56}, a sharp peak near 10keV appears in JENDL-4.0, but not in ENDF-7.1. 7) For Na^{23} capture and inelastic, large STD differences between JENDL-4.0 and ENDF-7.1 evaluators.

It was agreed the need for updated and complete covariance data. In this respect the feedbacks from CIELO are really important.

Finally, it was agreed that, if no other comments were made on the Ishikawa study, that will be finalized as partial deliverable for SG39.

5. Methodology

K. Yokoyama presented the work done on Action 7 (Methodology studies to avoid compensation, to point out to systematic effects, etc…). First, definitions of parameters/indices, and premises are introduced. Then, the assessment of adjustment is formulated. This assessment includes the selection of experiments and the detection of unreliable adjustments. It was also explained the static and dynamic methods for avoiding compensation effects. Finally, it is emphasized the importance of the "a posteriori" correlations since they come from combination of two physical data, i.e. differential and integral experiments.

G. Palmiotti presented the "PIA: Progressive Incremental Adjustment". This methodology is introduced as an approach for avoiding compensations (e.g. reaction variations of the same or different isotopes, lack of reactions and cross-correlations, inadequate covariances) and giving more reliable feedback to evaluator. A comparison with Global Adjustments is presented showing a significant impact on both central values and standard deviations. The work is focused on Na^{23}, Fe^{56}, $U^{238,235}$ and Pu^{239}. The PIA is applied in four steps: fission spectral indices, capture spectral indices and irradiation experiments, keff and reactivity step. Somme recommendations are made to produce trustworthy feedback to the CIELO evaluators, From CIELO; it is required good 'a priori' evaluations, with reliable and complete covariances. Selecting reliable experiments to avoid compensations, and/or identify new ones is a crucial mission for SG39. It was noted that βeff could be added to this adjustment.

A. Hoefer presented the MOCABA system, a general Monte Carlo-Bayes procedure for improved predictions of integral functions of nuclear data. In this scheme, NUDUNA samples/draws arbitrary nuclear data evaluation using the standard uncertainty MFs (MF31, MF32, MF33,…) within evaluated nuclear data. MOCABA system includes information of any kind integral observables (e.g. reactor power distribution, keff, …) without adjustment of nuclear data. More detailed information can be found in: http://arxiv.org/abs/1411.3172. New ideas of using MOCABA for updating of nuclear data libraries are currently under study.

E. Ivanov presented a sensitivity computation with Monte Carlo methods applied to FLATTOP-Pu, FLATTOP-25, ZPR-9/34, and ZPR-6/10 (Action 8). The objective is to test continuous energy (CE) and continuous angular distribution sensitivity capabilities implemented in Monte Carlo codes (MONK, SERPENTv2-IFP(Iterated Fission Probability), SCALE6.2B-IFP and CLUTCH, MCNP6-IFP). Also deterministic methods were used (SCALE6.1, ANISN/PARTISN). Some issues were observed: 1) large differences in U^{235} inelastic profiles for ZPR 9/34 were observed, 2) a spread of Fe^{56}-elastic sensitivity values for ZPR 6/10. Also, it was discussed the important role that convergence issues play in these problems. As general remarks: a good agreement between deterministic and all MC sensitivities is observed for nu-bar, fission, and capture profiles. In general, all tested MC methods and codes demonstrate consistency in the results that confirms the methods maturity. However, it has also been pointed out that MC scattering sensitivities depend on statistical options.

It was also concluded that the use of βeff for adjustment should be further investigated since it shows specific sensitivity profiles. A wide range of βeff experiments in France, USA, Germany, could be made available and the experimental uncertainties should be revisited if possible.

6. Data archive, plots etc.

O. Cabellos presented the status of online plots' comparison performed by E. Dupont. This info is available at NEA website: https://ww.oecd-nea.org/science/wpec/sg39/adjustment/results. Comments and feedbacks of SG40/CIELO meeting were discussed. CIELO´s proposal of a "CIELO/C" file including adjustments from SG39 is welcome and accepted by this SG.

7. Discussion, summary, next steps

The following list of actions was agreed.

Deliverables:

1- Methodology: summary to be prepared by M.Ishikawa and K.Yokoyama (finalized by May 2015)
2- Comments on covariance data: existing report by K.Y and M.I: make final comments if required (All). May 2015?
3- Sensitivity coefficients (MC vs deterministic + comments of potential issues with MC). State-of-the-art (KENO, SERPENT, MCNP6, TRIPOLI,…), recommendations.
E. Ivanov (leader) + I.Kodeli + PSI. Draft by May 2015

New experiments:

Actions:

- Neutron propagation experiments (FNS, FNG, JANUS): S.Pelloni, I.Kodeli, others (Analysis volunteers are needed)?? Experiment for O-16 to be analysed (I.Kodeli)
- Transmission (U-238, Fe): G.P will look into RPI transmission experiments.
- βeta effective: Methodology issues using βeff in adjustment, revision of past experiments, sensitivity profiles: I.Kodeli, PSI, E.Ivanov, (JAEA for comments/criticism/suggestions). BERENICE exp, CEA contribution? A summary to be presented by next meeting (see below)
- Oscillation experiments (STEK, SEG). Sensitivity profiles, C/E with associated uncertainties. What could be made available by NRG for STEK? (Da Cruz). INL exploratory study for SEG, other contribution? ERMINE experiments: CEA contributions? A summary on these actions to be discussed at next meeting (see below).
- PROTEUS (Ass> 7 and 8). Sensitivity profiles, C/E values. Available from PSI? Answer expected in the next few months (see also below)
- To extend the initial list of isotopes of interest for SG39, a priority list of isotopes (Fe^{56}, …, Am^{241}, …, Pd^{105},…) and associated experiments will be provided by Pino by next meeting

It was agreed that the following data for each of the experiments above, if made available should be delivered to the SG39 (Formats of SG33, 33 groups) (by May 2015):

- Benchmark model if available
- C/E with experimental uncertainties and correlations if applicable
- Sensitivity coefficients for isotope/reactions as for SG33 (+ possibly Am-241, Pd-105, O-16). Sensitivity coefficients should be provided for all significant isotopes
- Infinite dilution cross sections (SG33 format), i.e. spectrum independent.

Action on the evaluation of keff uncertainties for a simple case of Am^{241} using different codes and evaluated files. (I.Kodeli, other volunteers)

Reporting of actions, issues and feedbacks between SG39 and SG40 will be done, (e.g. for the case of O^{16}: processing of covariances). (O.Cabellos)

8. Next meeting

It is proposed to hold the next SG39 meeting in conjunction with WPEC/Subgroups meetings during the 27th WPEC Meetings at the NEA, May 19-20, 2015.

Appendix 1

Participants to the 3rd meeting of WPEC subgroup 39

NEA, Issy-les-Moulineaux, France

27-28 November 2014

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Appendix 2

Agenda of the 3rd meeting of WPEC subgroup 39

NEA, Issy-les-Moulineaux, France

27-28 May 2014

WPEC SG39

"Methods and approaches to provide feedback from nuclear and covariance data adjustment for improvement of nuclear data files"

	Thursday, November 27, 2014 **NEA Room B**	
13:30 – 13:45	**Welcome (G.Palmiotti, M.Salvatores, Oscar Cabellos)**	
13:45 – 14:30	**Sensitivity methods** • Sensitivity methods for SERPENT, M. Aufiero • Sensitivity code comparison for the SNEAK 7A/7B measurement analysis, I. Kodeli	
14:30 – 16:30	**Integral experiments** • PROTEUS experiments: selected experiments sensitivity profiles and availability, M. Hursin, M. Salvatores • Neutron propagation experiments o FNS Oxygen benchmark, I.Kodeli o Proposals and volunteers for re-analysis (ASPIS etc), I. Kodeli? , S. Pelloni?, G. Aliberti? • STEK (variable spectrum hardness experiments for FP) re-analysis, D. Da Cruz • SEG (tailored adjoint flux shapes), M.Savatores (comments) • IPPE transmission experiments (Fe, 238U), T.Ivanova? • RPI semi-integral (Fe, ^{238}U), G.Palmiotti (comments) • New experiments, e.g. in connection with the new NSC Expert Group on "Improvement of Integral Experiments Data for Minor Actinide Management": G.Palmiotti (Some comments from the Expert Group) • Discussion on possible contributions to the analysis	
16:30 – 17:30	**Integral experiments** • Additional PSI adjustment studies accounting for nonlinearity, S. Pelloni • Others? CEA?	
17:30	**Adjourn**	

	Friday, November 28, 2014 **NEA Room B**	
9:00 – 9:45	**Am-241 and fission product issues** • Am-241 validation for criticality-safety calculations, A. Barnes (Visio-conference) • Isotopes to be investigated by SG39, G.Palmiotti, all	
9:45 – 10:30	**Covariance data** • Any new validation, improvement study, P. Archer? • Analysis presented by K. Yokoyama at last meeting, if agreed, will be part of final report (K. Yokoyama comments) • Need for new and complete covariance data. Feedback from CIELO expected (?)	
10:30 – 10:45	***Break***	
10:45 – 12:30	**Methodology** • Methodology studies: summary, K. Yokoyama, G. Palmiotti • PIA: Progressive Incremental Adjustement, G.Palmiotti • NUDUNA / MOCABA: Monte Carlo-Bayes procedures for improved predictions of integral functions of nuclear data, A. Hoefer • FLATTOP-Pu, FLATTOP-25, ZPR-9/34, and ZPR-6/10 MC sensitivities, E. Ivanov et al.	
12:30 – 13:45	***Lunch Break***	
13:45 – 14:30	**Data archive, plots etc.** • Update on comparison plots (Databank: O. Cabellos)	
14:30 – 15:30	**Next steps** • Discussion (All); deliverables, final report • Availability of volunteers for new/dedicated integral experiment analysis (All) • Next meeting	
15:30	**Adjourn**	