Summary Record of the 1st (formal) 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

28-29 November 2013

The subgroup co-ordinators, **M. Salvatores** and **G. Palmiotti**, welcomed the participants to this formal kick-off meeting of the new WPEC Subgroup 39 (see list of participants in Appendix 1). The proposed agenda was adopted (see Appendix 2).

M. Salvatores reminded the participants of the subgroup objectives described in the mandate, which was approved by the WPEC in May and endorsed by the Nuclear Science Committee in June 2013. The structure of WPEC requires the nomination of subgroup monitor(s) and **M. Ishikawa** accepted to be one of them. The second monitor would have been **R. McKnight** who was monitoring SG33 and one of the main initiators of this activity. Dick passed away in August 2013 and will be greatly missed.

E. Dupont mentioned that the mandate is available on the SG39 webpage and that all materials discussed within the framework of this subgroup will be made publicly available on the web, unless explicitly requested by the author(s) that the access should be password protected.

1. Recent data adjustments performances and trends (for ^{235}U, ^{238}U, ^{239}Pu, ^{56}Fe and ^{23}Na)

M. Ishikawa summarized preliminary recommendations for ^{239}Pu, ^{238}U, ^{235}U, ^{56}Fe and ^{23}Na data inferred from a large adjustment study performed at JAEA (ADJ2010, cf. JAEA-Research 2012-013, JAEA, July 2012[*]). He highlighted the good performance of the current JENDL-4.0 data for ^{239}Pu fission and nu-bar, and for the capture cross sections of ^{235}U and ^{238}U. Additional work will be necessary to understand adjustment trends for ^{235}U fission, ^{239}Pu capture cross section and fission spectrum, and for the scattering cross sections of ^{23}Na, ^{56}Fe, ^{238}U and ^{239}Pu.

G. Palmiotti reported on feedback on the Big-3 actinide data inferred from the ENDF/B-VII.0 adjustment study. The ^{235}U, ^{238}U and ^{239}Pu inelastic cross sections are all reduced in the range ~1-5 MeV. The ^{235}U and ^{238}U capture cross sections do not change too much, but the ^{239}Pu capture cross section is significantly reduced (5 to 10%) from 1 keV to 10 keV. The (n,2n) cross section is reduced for ^{238}U, whereas it is significantly increased for ^{239}Pu. There is no major adjustment of the fission cross sections because the evaluated uncertainties are very low.

I. Kodeli reported on additional studies of FLATTOP-Pu sensitivities using SUSD3D/PARTISN, SUSD3D/ANISN and ERANOS with different anisotropy orders (P_N). The sensitivity profiles of k_{eff} to the ^{238}U scattering cross sections are similar when using the higher orders (P_3, P_5), but significant differences can be seen if the calculations are limited to P_1.

[*] Available from JAEA at http://jolissrch-inter.tokai-sc.jaea.go.jp/search/

S. Pelloni presented the latest adjustment results performed at PSI using ERANOS with two different data sets (JEFF-3.1 + COMMARA-2.0 and ENDF/B-VI.8 + BOLNA). The results are consistent with trends observed in the SG33 benchmark.

E. Ivanov studied how to define a consistent set of integral benchmarks and associated correlations in order to perform reliable data assimilation. He showed examples of the impact of integral uncertainty correlations on the integral performance assessment of evaluated libraries, and provide recommendations to ensure the full consistency of the integral information.

M. Hursin presented an overview of the PROTEUS experimental programme performed at PSI over more than 30 years. In the 70's the Gas-Cooled Fast Reactor (GCFR) experiments were essentially designed to improve the nuclear data in the fast energy range. The light water reactor experiments performed in the 80's (HCLWR) and until 2006 (LWR-PROTEUS, Phases I, II and III) allowed to study various configurations for PWR and BWR. More information is available on the PROTEUS website at http://proteus.web.psi.ch.

J. Dyrda reported on the data assimilation of benchmark experiments for homogeneous thermal and epithermal uranium systems. The assimilation method is based on Kalman filters using integral parameters and sensitivity coefficients calculated with MONK9 and ENDF/B-VII data. The assimilation process results in an overall improvement of the calculation-benchmark agreement, and may help in the selection of nuclear data after analysis of adjustment trends.

2. Strategy for selection of devoted experiments (for ^{235}U, ^{238}U, ^{239}Pu, ^{56}Fe and ^{23}Na)

In addition to the bulk of integral experiments already used the issue is to select (and calculate) additional integral parameters that would focus more specifically on ^{235}U, ^{238}U, ^{239}Pu, ^{56}Fe and ^{23}Na nuclear data.
M. Salvatores made a list of integral experiments already mentioned during the previous discussions: PROTEUS (PSI), BERENICE (Cadarache), STEK (Petten), SEG (Rossendorf), FLATTOP w/wo reflector, neutron transmission through Na, Fe, e.g. ASPIS (Winfrith).
T. Ivanova inquired about the possibility to cover the thermal and epithermal ranges. **M. Salvatores** agreed providing that suitable experiments could be used. **T. Ivanova** proposed to make a list of relevant thermal benchmarks, but said that it would be more difficult for epithermal data.

3. Methodology issues:

G. Palmiotti reviewed the various adjustment methodology issues that the subgroup should address to provide reliable feedback. For example: (1) Criteria to help select or eliminate integral experiments and to assess adjustment results, e.g. Adjustment Margin (AM) and Experiment Merit (EM) already used in the SG33 benchmark, total and individual chi-squares, etc.; (2) Criteria to assess nuclear data adjustments, e.g. consistency with nuclear data uncertainty range, comparison with other evaluated files; (3) Problem of compensation in the adjustment of nuclear data due to missing reaction(s) or wrong estimation of prior uncertainties. Some solutions were proposed and discussed by the participants.

C. De Saint Jean reported on nuclear data activities at CEA Cadarache, e.g. marginalisation techniques to account for systematic uncertainties, use of Lagrange multipliers to impose simultaneous consistency constraints on several models, assimilation of integral data during the evaluation process, adjustment of nuclear reaction model parameters, evaluation of covariance matrices, etc. The CEA activities cover both differential and integral data and the possible synergies between SG39 and SG40-CIELO were highlighted. These two new subgroups have the potential to link evaluation and integral experiments beyond the traditional validation issues.

G. Palmiotti reported on the consistent adjustment of nuclear data parameters performed within a BNL-INL collaboration. The main advantage compared to the classical adjustment of multigroup constants is to provide final nuclear data constrained by the nuclear reaction theory and consistent with both differential and integral measurements. The feasibility of a single-isotope assimilation was tested on a few priority materials (^{23}Na, ^{56}Fe, ^{105}Pd, ^{235,238}U, ^{239}Pu) using a selection of clean integral experiments. The multi-isotope assimilation is under study for the Big-3 (^{235,238}U, ^{239}Pu). This work showed that a consistent assimilation is feasible, but there are pitfalls to avoid (e.g. non-linearity, cross section fluctuations) and prerequisites (e.g. realistic covariances, good prior, realistic weighting of differential and integral experiments). Finally, only all experimental information combined with the state of the art modelling may provide a "right" answer.

4. Discussion, summary, next steps, actions

The following conclusions summarise the meeting discussions, issues and actions.

C1. Compensations in current adjustments (see example by M. Ishikawa: case of ^{239}Pu Chi, ^{23}Na(n,n'), ^{238}U(n,n') and ^{239}Pu(n,n')). There is a need for integral experiments able to discriminate between these effects, see point C7 below for a few suggestions. The analysis of current adjustments trends can also help (see point C6 below). In addition, there is a need for covariance data as complete and reliable as possible (this is an item for discussion with CIELO evaluators in May).

C2. Adjustment of ^{235}U data: are there enough experiments accounted for? More experiments are certainly needed to improve the high energy range.

Action on all: to suggest additional integral experiments sensitive to ^{235}U.

C3. Energy range of interest. At present the range 500 eV – 5 MeV is fairly well covered. There is a need for additional experiments to cover thermal and epithermal spectra.

Action on T. Ivanova and M. Hursin: to suggest integral experiments for the thermal and epithermal energy range (e.g. PROTEUS- HCLWRs?)

C4. Role of integral β_{eff} measurements in the adjustment of delayed neutrons (and availability of related nuclear data covariance).

Action on I. Kodeli, E. Ivanov, M. Ishikawa (for deadline see point C7 below): to look into BERENICE experiments and ANL β_{eff} experiments (accuracy, relevance etc.).

C5. Secondary neutron distribution adjustment: need sensitivity and covariance data.

C6. As for already existing adjustments (JAEA, CEA, INL, PSI, IRSN…), it is proposed to compare adjusted cross sections of the five isotopes (^{239}Pu, ^{235}U, ^{238}U, ^{56}Fe and ^{23}Na) in 33 groups, using SG33 format. The prior and posterior uncertainties should be reported too. The standard values should be included in the comparison. This comparison and associated analysis could be the basis for an interim report to CIELO by May 2014. Two hypotheses: a) discuss results and iterate by email, b) make discussion in May 2014. In that case, the meeting with CIELO would be in November 2014.

Action on C. De Saint Jean, M. Ishikawa, G. Palmiotti, S. Pelloni, T. Ivanova, E. Ivanov, E. Dupont: to prepare this comparison.

C7. Specific integral measurements can be required in order to avoid as much as possible compensation effects and provide valuable information on separated effects:

- Single isotope (e.g. sample irradiation effects for capture and (n, 2n) cross-sections). However, few experiments are available.

- Neutron propagation experiments for elastic/inelastic scattering cross sections, e.g. ASPIS iron propagation experiment. Action on I. Kodeli: to report on existing propagation experiments.
- "Flat" adjoint flux experiments (to separate inelastic from absorption cross sections). The STEK experiments have been documented in a JAEA report and a reanalysis is underway at Petten. Any other experiment of this type available? Action on E. Dupont, E. Ivanov, M. Ishikawa, M. Salvatores: to look into these experiments and see if they could be useful for the present purposes.
- ^{238}U sphere neutron transmission experiments (e.g. Obninsk experiments). Others? Action on T. Ivanova, C. De Saint Jean, G. Palmiotti: to look into these experiments.

Action on G. Palmiotti, M. Salvatores, M. Ishikawa, E. Ivanov, T. Ivanova, C. De Saint Jean, I. Kodeli, S. Pelloni, M. Hursin: to prepare a summary by the next meeting (May 2014) on all these experiments (see also points C2, C3 and C4) with preliminary documents to be circulated ahead of that date for comments.

C8. The scattering anisotropy (P_N) needs to be carefully accounted for (cf. FLATTOP case analysed by I. Kodeli). In this frame, new full MC methods have been developed and should be compared, e.g. on the same FLATTOP experiment (Action on E. Ivanov).

C9. Methodology issues

- Adjusted central values acceptability: if it stays in ~1sigma of original uncertainty.
- Adjustment in low sensitivity energy regions: acceptable if correlations in energy do require them.
- Experiment "rejection": better use the different criteria for giving "warnings". Criteria to be summarized (Action on G. Palmiotti).
- Use of a posteriori covariance data: if feedback to designers, both adjusted data and a posteriori covariance; if feedback to evaluators, only trends will be given. The method to avoid generation of not previously existing cross correlations could be suggested (Action on E. Ivanov, T. Ivanova).
- Prepare a list of priority missing covariance data types (see also points C4 and C5) and list of "suspect" low values (file dependent) (Action on M. Ishikawa). This list will be discussed with CIELO evaluators.
- Nuclear parameter adjustment: first attempts promising. However not yet consensus. Needs some further discussion and iteration with evaluators.

Action on G. Palmiotti, C. De Saint Jean, E. Ivanov, M. Ishikawa, M. Salvatores: to prepare a summary of methodology issues for further discussion at next meeting (May 2014).

5. Next meeting

It is proposed to hold the next SG39 meeting in conjunction with other subgroup meetings during the WPEC week (May 12-16, 2014). One full day should be devoted to a joint meeting with the SG40-CIELO Subgroup.

Appendix 1

Participants to the 1st (formal) meeting of WPEC subgroup 39

NEA, Issy-les-Moulineaux, France

28-29 November 2013

C. De Saint Jean	CEA, France	
E. Dupont	NEA, OECD	(Secretary)
J. Dyrda	AWE, UK	
M. Hursin	PSI, Switzerland	
M. Ishikawa	JAEA, Japan	(Monitor)
E. Ivanov	IRSN, France	
T. Ivanova	IRSN, France	
D.H. Kim	KAERI, Korea	
I. Kodeli	JSI, Slovenia	
L. Leal	ORNL, USA	
Y.-O. Lee	KAERI, Korea	
D. Leichtle	F4E, Spain	
G. Palmiotti	INL, USA	(Coordinator)
S. Pelloni	PSI, Switzerland	
V. Pronyaev	IPPE, Russia	
M. Salvatores	INL, USA	(Coordinator)
S. Simakov	IAEA, Austria	

Appendix 2

Agenda of the 1st (formal) meeting of WPEC subgroup 39

NEA, Issy-les-Moulineaux, France

28-29 November 2013

Thursday 28, pm

1- Introduction, objectives, mandate, agenda, etc.

2:00 pm (M.Salvatores, G.Palmiotti)

Recent data adjustments performances and trends for Pu-239, U-238, U-235, Fe-56 and Na-23, in view to organize a first summary (deadline ~May 2014) to be submitted to CIELO

2:15 pm Recommendations from ADJ2010 Adjustment (M.Ishikawa)

2:45 pm Feedback on CIELO Isotopes from ENDF/B-VII.0 Adjustment (G.Palmiotti)

3:15 pm Break

3:30 pm Sensitivity and Uncertainty Results on FLATTOP Pu (I.Kodeli)

3:45 pm SG33 Benchmark: Comparative Adjustment Results (S.Pelloni)

4:00 pm Integral benchmarks for data assimilation: selection of a consistent set and establishment of integral correlations (E.Ivanov)

4:30 pm Any other contribution

2- Strategy for selection of devoted experiments for CIELO isotopes and validation of related adjusted uncertainties. Further adjustment work expected

5:00 pm Discussion (All)

5:30 pm Adjourn

Friday 29, am

9:00 am PROTEUS experimental data (M.Hursin)

9:30 am Data assimilation of benchmark experiments for homogeneous thermal and epithermal uranium systems (J.Dyrda)

3- Methodology issues:

- **How to choose integral experiments and how to detect anomalies**
- **Missing experiments**
- **Validation of correlation matrices. Features to be improved**
- **Parameters to be adjusted beyond neutron cross sections: angular distributions, secondary neutrons energy distributions etc.**
- **How to possibly detect compensations**
- **A-posteriori correlation matrices**
- **Nuclear data parameter adjustment**
- **Others**?

10:00 am Introduction and preliminary discussion (M.Salvatores, all)

10:30 am Methodology Issues, INL (G.Palmiotti)

11:15 am Break

11:30 am Marginalisation, Methodology Issues, and Nuclear Data Parameter Adjustment, CEA (C.De Saint Jean)

12:15 pm Nuclear Data Parameter Adjustment, BNL-INL (G.Palmiotti)

1:00 pm Lunch Break

Friday 29, pm

4- Discussion, summary, next steps, definition of deliverables

2:00 to 3:00 pm All

3:00 pm Adjourn