Summary Record of the 4th Meeting of the WPEC Subgroup 33 on

Methods and issues for the combined use of integral experiments and covariance data

NEA, Issy-les-Moulineaux, France

29-30 November 2010

The subgroup coordinators, **M. Salvatores** and **G. Palmiotti**, opened the meeting and welcomed the participants (cf. list in Appendix 1). Participants from France (IRSN), Switzerland (PSI), and Korea (KAERI) joined Sg33 activities recently and attended the meeting as observers.

The proposed agenda was adopted (cf. Appendix 2). **M. Salvatores** reminded the participants of the objectives of the benchmark and reviewed the actions of the previous meeting.

1. Report on adjustment methodologies

A draft version of the report on adjustment methodology was sent to Sg33 members in October 2010. Comments on this draft version and proposal for modifications were discussed by the participants during the meeting. **E. Dupont** will include all corrections in the final version and will circulate it again among Sg33 members before publication by the NEA (Action 1).

2. Status of integral experiments

2.a. Corrective Factors Dependence from Cross Section Data Sets

G. Palmiotti repeated the calculation of corrective factors using two different evaluated libraries (ENDF/B-VII.0 and ENDF/B-VI.8) in order to assess the dependence on data sets. The impact on corrective factors is generally small, i.e. of the order of a few tens of pcm on k_{eff} and on a few tenths of percent on spectral indices. A difference of 130 pcm between the two libraries was observed in the case of FLATTOP and requires further investigation. Nevertheless, this value could be added as extra uncertainty on the C value. G. Palmiotti also stressed that a different corrective factor was obtained for FLATTOP k_{eff} using ENDF/B-VII.0 compared to the previous results. New corrective factors will be distributed (Action 2).

R. McKnight commented that ENDF/B-VI.8 and ENDF/B-VII.0 are rather close and this could also explain the small impact on corrective factors. **T. Ivanova** mentioned the existence of a benchmark to evaluate the effect of homogeneous vs. heterogeneous calculations. This benchmark is coordinated by the NEA WPNCS expert group on Uncertainty Analyses for Criticality Safety Assessment (UACSA).

G. Palmiotti presented one more slide on the status of calculated (C) and experimental (E) values and associated uncertainties for all benchmark experiments. He highlighted the rather large uncertainties assigned to the calculated values of the two ZPPR9 Na void configurations. He also inquired about possible revision of the experimental uncertainty of some ICSBEP benchmarks.

M. Ishikawa confirmed these uncertainties and explained that Na voids are very difficult to calculate accurately. **R. McKnight** said that a proposal has been made to increase the k_{eff} experimental uncertainty of JEZEBEL (Pu-239) from 100 pcm to about 200 pcm.

2.b. Proposal for how to determine Error Matrix of Analytical Modelling

M. Ishikawa reminded the importance to estimate (and include in the equation if necessary) the covariance matrix relative to analytical modelling errors (V_m). Three cases were discussed depending on the type of calculations, (1) continuous-energy Monte Carlo (MC) simulation, (2) most-detailed deterministic calculation, (3) combination of MC and deterministic methods. In the first case (MC simulation), the uncertainties are purely statistical and provided by the MC code, whereas the uncertainty correlations can be neglected. However, on the basis of detailed statistical analysis of MC results, JAEA recommends to multiply the estimation of the standard deviation by a factor 2. In the second case (deterministic calculation), some assumptions are necessary to estimate both the uncertainties and their correlations, which cannot be neglected. In the third case (combination of MC and deterministic calculations), the uncertainties and their correlations would be estimated as in case 1 (MC) under the condition that the correction values are obtained through well-organized simulation models from the analytical modelling error viewpoint.

M. Salvatores agreed on the principle to estimate the analytical modelling errors and to include them in the adjustment, if necessary. After some discussions on the difficulty to estimate modelling uncertainties, it was decided that all k_{eff} reference calculations should be performed with as-built MC simulations and that the modelling uncertainty (1 σ) should be assumed as 2 times the statistical uncertainty (1 σ) calculated by the MC code (i.e. case 1). In addition, JAEA will provide an estimation of the full covariance matrix (V_m) relative to modelling errors of deterministic calculations (case 2). **M. Ishikawa** agreed to provide V_m associated to the deterministic calculations of ZPPR9 configurations.

2.c. Discussion on experimental and calculation uncertainties

M. Salvatores summarized the discussions on experimental and calculation uncertainties for integral data. **R. McKnight** will check experimental uncertainties of all integral benchmark values and provide new uncertainties if necessary (Action 3). ANL will provide MC model of ZPPR9 (Action 4). **G. Palmiotti** will perform as-built MC simulations of integral experiments selected for the benchmark exercise (JOYO included), and will circulate updated corrective factors and modelling uncertainties (Action 2). **M. Ishikawa** will further study the analytical modelling errors of deterministic calculations and provide an estimation of V_m for ZPPR9 configurations (Action 5). All participants will provide comments and feedback on the JAEA approach to evaluate method uncertainty (Action 6).

3. Status of covariance for nuclear data

3.a. AFCI-2.0β Covariance Library

S. Hoblit presented the status of the AFCI-2.0β covariance library. The initial purpose of this project was to provide reliable covariance data for nuclear data adjustment. The library contains covariance data (on cross sections, mu-bar, nu-bar, and prompt fission neutron spectra) for 110 materials relevant to fast reactor R&D (12 light nuclei, 78 structural materials, 20 actinides). The evaluation methodology was adapted to the importance of the material. The data for the 30 most important materials were evaluated using the most sophisticated methods. The data for 40 materials of medium importance were evaluated with simplified methods, whereas the evaluation of the remaining materials was based on low-fidelity approach. The AFCI-2.0β library is being tested under quality assurance and the final release is planned in December 2010. These data will be available to Sg33 members participating to the benchmark exercise (Action 7).

M. Ishikawa was concerned about the independent evaluation of covariance data and central values. **M. Herman** agreed on the principle. He added that although AFCI-2.0 covariance data are strongly linked to ENDF/B-VII.0 central values, most of them are expected to be still valid for the forthcoming ENDF/B-VII.1 library. Nevertheless, new covariance data evaluation will be performed for ENDF/B-VII.1 data that significantly differ from ENDF/B-VII.0.

3.b. Proposal to evaluate Nuclear Data covariances

M. Ishikawa made a proposal to assess covariance data within Sg33. He illustrates the discrepancy between uncertainty evaluations in major libraries on three important examples: Pu-239 fission, U-238 capture, and Na-23 inelastic cross sections. He outlined a procedure: 1) to compile and plot the nuclear data and their covariances used in the SG33 exercise, 2) to identify the discrepancies, 3) to initiate discussion with nuclear data physicists, and 4) to make final recommendations based on the user's viewpoint.

M. Salvatores found the proposal acceptable and actually similar to the procedure adopted within the AFCI project. However, Sg33 focus is on adjusted covariance data in order to reduce uncertainties on target design. Nevertheless, verification of prior covariance data is a part of the benchmark exercise and will be essential to understand differences between the results of phase I (own covariance data) and phase II (common covariance data).

4. Discussion on covariance data for integral experiments

The JAEA proposal (cf. June 2010 meeting) for integral experimental data uncertainties and their correlations was discussed by the participants. **R. McKnight** commented that the proposed uncertainties seem reasonable and similar to ICSBEP values. However, part of them may include modelling uncertainties as well (k_{eff} only, the model-dependent contribution to the spectral index uncertainties can be neglected). **R. McKnight** stressed that only pure experimental uncertainties should be considered if as-built MC simulations are performed.

M. Ishikawa recommended explaining Sg33 choices relative to integral experimental data uncertainties. **R. McKnight** agreed to peer-review the JAEA proposal and to document any proposal for modification (Action 3).

M. Salvatores and **R. McKnight** said that the uncertainty correlations seem reasonable and should be adopted. **M. Salvatores** added that the full covariance matrix could be peer-reviewed by IPPE as well (Action 8).

5. Uncertainty evaluation on the target systems

5.a. ABR and FBR Uncertainty Evaluation with AFCI-2.0

G. Palmiotti presented uncertainty calculations for the ABR and FBR cores (k_{eff} and sodium void in core regions) based on ENDF/B-VII.0 and AFCI-2.0β covariance data (cross sections only). ABR integral parameter uncertainties are affected by relatively large uncertainties on a few cross sections: U-238 capture and inelastic, Pu-239 capture and fission, Fe-56 scattering (for all integral parameters), and Na-23 inelastic (for Na void). In the case of FBR integral parameter uncertainties, there is one additional and significant contribution from the uncertainty of Pu-241 fission cross section. Indeed, the latter have been increased in AFCI-2.0β to reflect the large discrepancy (~25%) between old data and recent measurement performed at LANSCE.

5.b Nuclear Data Uncertainty Propagation: Preliminary Results

D. Rochman gave an overview of the preliminary results obtained at NRG. A progress report containing all results was distributed before the meeting. Sensitivity coefficients to k_{eff} have been calculated with MCNP for 7 benchmark experiments and target systems out of 9 (MCNP models are missing for ZPR6-7 and ABR). Covariance data from TALYS/TENDL have been propagated using these sensitivity coefficients to calculate k_{eff} uncertainties. TMC-based uncertainty calculations are ongoing and only partial comparison with results obtained with the perturbation method could be shown.

M. Salvatores commented that contributions of U-238 capture and Pu-239 nu-bar uncertainties on ZPPR9 k_{eff} uncertainty is very large and questioned the assumptions made to evaluate the former ones. **D. Rochman** answered that the uncertainty of Pu-239 nu-bar could be around 1% but this has to be confirmed.

5.c. Preliminary Results of the ZPR6-7 and ZPR9 S/U Analysis

I. Kodeli presented preliminary results of k_{eff} S/U analysis on ZPR6-7 and ZPR9[1] integral benchmark experiments. The analysis was performed with deterministic S_n codes and multigroup cross-section libraries available from the NEA Data Bank. The large C/E discrepancy observed for ZPR9 k_{eff} could be explained either by deficiencies in W or in U-235 and U-238 nuclear data. It was observed large differences between covariance data from various projects (e.g. SCALE, IRDF, JENDL) that could lead to very different adjustment results.

5.d. Preliminary Uncertainty Analysis at ANL

W.S. Yang presented preliminary S/U analysis of all benchmark experiments. The study was performed with MCNP and VIM for Monte-Carlo simulations and with TWODANT, VARIANT, and ERANOS for deterministic calculations and perturbation analysis. Sensitivity coefficients for fission spectra were obtained from direct calculations with ERANOS. Nuclear data from the ENDF/B-VII.0 library were used together with different versions of the AFCI covariance data. Integral parameter values and uncertainties calculated with different routes and different covariance data were compared. The major contributions to integral parameter uncertainty were highlighted in the case of FLATTOP k_{eff} and ZPPR9 Na voids.

6. Benchmark adjustment – Phase I

6.a. Status of CEA Activities

C. de Saint Jean presented preliminary adjustment results obtained with (preliminary) in-house covariance data. Integral parameters and associated sensitivity coefficients to nuclear data (including nu-bar and fission spectrum) have been calculated with the ERANOS/PARIS code and JEFF-3.1.1 data. A conventional multigroup adjustment was performed in the CONRAD framework. Preliminary results show a reduction by a factor 5÷10 of the integral parameter uncertainties due to nuclear data. The related reduction on the "usual suspect" uncertainties is by a factor 3÷6 for Pu-239 fission and U-238 capture cross sections.

6.b. Adjustment Phase I – INL Preliminary Solution

G. Palmiotti presented preliminary adjustment results obtained with AFCI-2.0β covariance data. Integral parameters have been calculated with MCNP or ERANOS (for ZPPR9 and JOYO) using ENDF/B-VII.0 data. All sensitivity coefficients have been calculated with the ERANOS code system. Significant improvements in the C/E ratio after adjustment are obtained for the k_{eff} of ZPPR9 and JOYO, the F28/F25 spectral index of ZPR6-7 and ZPPR9, and for ZPPR9 Na voids. The related changes in nuclear data involve mainly U-238 inelastic and U-235 capture (for JOYO), as well as Pu-239 capture and Fe-56 inelastic cross sections.

T. Ivanova commented that one should be careful if significant nuclear data adjustment were obtained in region where self-shielding would not be negligible. **G. Palmiotti** answered that this should not occur with the present selection of fast benchmarks. **M. Salvatores** added that iterations would be possible in order to converge on the adjustment of infinite dilution cross sections.

[1] The ZPR9 experiment is not part of the benchmark exercise (unlike Z<u>PP</u>R9) but can be considered for the verification of the adjustement procedure.

6.c. Benchmark Results by JAEA

K. Sugino presented adjustment results performed with JENDL-4.0 nuclear data and covariance. Integral parameters have been calculated with continuous-energy Monte Carlo (MC) method. The analytical modelling uncertainty was included in the adjustment and assumed equal to the statistical uncertainty of the MC result. Changes in C/E values of benchmark experiments and target systems, as well as related adjustment of cross sections were presented with and without taking into account the analytical modelling uncertainty. It was stressed that the analytical modelling error should be adequately considered in the adjustment.

7. Future steps

A priority in view of next meeting is the completion by the participants of the adjustment exercise and the distribution of the associated results according to the agreed formats (Action 9).

Comparisons of covariance data sets and available adjustments will be prepared by the Secretariat (Action 10).

8. Next meeting

The next meeting will be held at the NEA, Issy-les-Moulineaux, France on 10-11 May 2011 in conjunction with JEFF and WPEC meetings.

9. Actions

1.	E. Dupont	To include all modifications and circulate among Sg33 members the final report on adjustment methodology. To publish the report on adjustment methodology as a NEA/NSC document.
2.	G. Palmiotti	To check corrective factors for FLATTOP. In general to provide consolidation of procedure to define correction factors and circulate document early 2011. To increase by a factor 2 the uncertainty of as-built MC calculations. To circulate up-to-date description of benchmark specifications.
3.	R. McKnight	To check the integral uncertainties (e.g. ZPR6-7) and correlations proposed by JAEA and document any proposal for modification (early 2011, before next meeting).
4.	W.S. Yang R. McKnight	To provide MC model of ZPPR-9.
5.	M. Ishikawa	To further study the analytical modelling error of deterministic calculations and provide an estimation of V_m for ZPPR9 configurations.
6.	All	To provide comments and feedback to JAEA on the method uncertainty approach (by February 2011).
7.	M. Herman	To release, by the next meeting, AFCI 2.0 covariance data to Sg33 members for the benchmark exercise.
8.	M. Salvatores	To contact IPPE and ask them to peer-review the integral uncertainties and their correlations to be used in the benchmark exercise.
9.	All	To complete the phase I of the benchmark adjustment exercise and distribute the data in the agreed format.
10.	E. Dupont	To collect input/output data from the phase I benchmark and prepare them for comparison.
11.	E. Dupont	To update the subgroup web page with materials from this meeting and other participant contributions.

Appendix 1

Participants to the 4th meeting of WPEC subgroup 33

NEA, Issy-les-Moulineaux, France

29-30 November 2010

M. Salvatores	INL, USA – CEA, France	(Coordinator)
G. Palmiotti	INL, USA	(Coordinator)
R. McKnight	ANL, USA	(Monitor)
E. Dupont	NEA, OECD	(Secretary)
M. Herman	BNL, USA	
S. Hoblit	BNL, USA	
M. Ishikawa	JAEA, Japan	
T. Ivanova	IRSN, France	
S.-J. Kim	KAERI, Korea	
I. Kodeli	IJS, Slovenia	
S. Pelloni	PSI, Switzerland	
M. Pigni	BNL, USA	
D. Rochman	NRG, Netherlands	
C. de Saint Jean	CEA, France	
K. Sugino	JAEA, Japan	
W.S. Yang	ANL, USA	

Appendix 2

Agenda of the 4th meeting of WPEC subgroup 33

NEA, Issy-les-Moulineaux, France

29-30 November 2010

Monday 29 November

1) 13:30 – 14:30 **Welcome, approval of the agenda. Deliverables.**

a. Discussion and finalisation of Report/Deliverable on Adjustment Methodologies.

2) 14:30 – 16:30 **Status of integral experiments**

a. Corrective Factors Dependence from Cross Sections Data Sets, G. Palmiotti
b. Proposal for how to determine Error Matrix of Analytical Modelling, M. Ishikawa
c. Discussion on experimental and calculation uncertainties

3) 16:30 – 17:30 **Status of covariance for nuclear data**

a. AFCI-2.0β Covariance Library, S. Hoblit
b. Proposal to evaluate Nuclear Data covariance in Sg33, M. Ishikawa

Tuesday 30 November

4) 9:00 – 10:00 **Covariance data for integral experiments**

a. Discussion on integral uncertainties and their correlation, R. McKnight

5) 10:00 – 12:30 **Uncertainty evaluation on the target systems**

a. ABR and FBR Uncertainty Evaluation with AFCI-2.0, G. Palmiotti
b. Nuclear Data Uncertainty Propagation: Preliminary Results, D. Rochman
c. Preliminary Results of the ZPR 6-7 and ZPR-9 S/U Analysis, I. Kodeli

5) 14:00 – 15:00

d. Preliminary Uncertainty Analysis at ANL, W.S. Yang

6) 15:00 – 16:00 **Phase I Adjustments**

a. Status of CEA Activities, C. de Saint Jean
b. Adjustment Phase I – INL Preliminary Solution, G. Palmiotti
c. Benchmark Results by JAEA, K. Sugino

7) 16:00 – 16:30 **Future steps**