Summary Record of the 5th 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

11 May 2011

The subgroup coordinators, **M. Salvatores** and **G. Palmiotti**, opened the meeting and welcomed the participants (see Appendix 1). Sg33 members from China (CIAE) attended the meeting for the first time and additional WPEC members from Russia, USA and Japan were also present as observers.
The proposed agenda was adopted with the addition of one item to clarify the use of corrective factors (see item number 6 on *The use of corrective factors* by **G. Palmiotti**) and two more talks by **R. McKnight** (under item number 8 on *Uncertainty evaluation*) and **C. de Saint Jean** (under item number 9 on *Adjustment exercise*). The final agenda is available in Appendix 2. **M. Salvatores** reviewed the actions of the previous meeting. An updated list of actions is available at the end of this document (see section 11).

1. Discussion on progress of Sg33 activities and release of first deliverable

M. Salvatores reminded the participants of the benchmark objectives, which are to study the convergence of adjustment methods, the impact of different cross-section and/or covariance data input and to assess the consistency of reduced uncertainties. The initial assessment of adjustment methodologies used by the participants has been completed and the results published by the NEA[1]. A set of integral experiments has been selected and calculated by all participants. **M. Salvatores** stressed the importance of this intermediate step and recommended that all integral uncertainties and associated documents be preserved together with participant's calculated values. The first phase (out of three) of the benchmark exercise is ongoing and preliminary adjustment results are already available using each participant's covariance data. A new set of covariance data (COMMARA) has just been released by BNL and will be used in the second phase of the benchmark exercise by all participants.

2. Adjustment methodology

H. Wu presented the current status of CIAE/CNDC activities on nuclear data adjustment. In the past, a few CENDL evaluations have been fine tuned on the basis on trends from integral benchmark results. However, CNDC has no experience in multi-group cross-section adjustment. Participation to the Sg33 benchmark exercise will contribute to develop S/U analysis (1D for the moment) and nuclear data adjustment capabilities at CIAE/CNDC. Preliminary calculations of benchmark integral experiments were presented for Jezebel, Flattop and ZPR6-7. Work is ongoing to complete the first phase of the benchmark exercise.

[1] "Assessment of Existing Nuclear Data Adjustment Methodologies", International Evaluation Co-operation, NEA/WPEC-33, Intermediate Report, NEA/NSC/WPEC/DOC(2010)429, OECD Nuclear Energy Agency, 2011.

S. Pelloni commented that preliminary integral experiment calculations are consistent with PSI results except for ZPR6-7 values, which differ significantly. **R. McKnight** noted that different benchmark models could explain this discrepancy.
G. Palmiotti commented that S/U analysis of Na void experiments will require 2D calculations.

3. Integral experiment analysis

R. McKnight updated the participants with the latest analysis of the ZPPR-9 integral experiments. Some discussions followed about the difficulty to calculate accurately Na voids using Monte-Carlo methods. Indeed, the computer time required to reduce the statistical uncertainty below an acceptable level ranges from one week to one month depending on the code used. **G. Palmiotti** concluded that reactivity coefficients are usually difficult to calculate with Monte Carlo codes.

4. Cross section covariance matrix

4.a) W. Wang presented ongoing work at CIAE/CNDC relative to the Sensitivity/Uncertainty analysis of integral parameters. Development of S/U tools has just started, but basic S/U analysis is already possible with the SENS(1D) code complemented with the NJOY and SCALE systems. Future plans include comparison with other deterministic codes and MCNP results, use of different data library, influence of self-shielding, 2D and 3D calculations, as well as S/U analysis for burnup.

T. Ivanova commented that the current version of MCNP is not satisfactory for sensitivity calculations and that a benchmark for *calculation of k_{eff} sensitivity to neutron cross sections* is in preparation in the framework of the NEA/WPNCS Expert Group on Uncertainty Analysis for Criticality Safety Assessment (UACSA). More information is available under item 7.
G. Palmiotti noted that calculations to be performed in the benchmark exercise require 2D S/U tools for Na voids and implementation of the Generalized perturbation theory (GPT) for reaction rates. **M. Salvatores** suggested compiling a list of the most useful references related to the S/U analysis methodology and to make it available to Sg33 members (Action 1).

4.b) M. Herman announced the release of a set of Covariance multigroup matrix for advanced reactor applications (COMMARA-2.0). The name was changed from AFCI to COMMARA but the numbering was kept to avoid confusion in the version. In comparison with AFCI-2.0β, presented at the Sg33 November 2010 meeting, AFCI/COMMARA-2.0 includes recent LANL actinide covariance data and revision of ^{241}Pu fission uncertainties. The COMMARA-2.0 data are available to all Sg33 members for the phase II of the benchmark exercise.

M. Ishikawa noted that covariance data for the average cosine (mu-bar) of elastically scattered neutrons on ^{238}U were missing in COMMARA-2.0. **M. Chadwick** commented that the prompt fission neutron spectrum of ^{235}U could be added as well. **M. Ishikawa** proposed to use JENDL data for the benchmark exercise, if necessary. **M. Salvatores** agreed with this proposal pending verification of consistency issues.

5. Integral experiment covariance matrix

5.a) M. Ishikawa reminded the participants about the JAEA proposal for the integral experiment covariance data (see Sg33 June 2010 meeting). After peer-review by **R. McKnight** the integral experiment uncertainties were adopted. **M. Salvatores** questioned the large correlation (0.5) assumed between Na void measurements. **M. Ishikawa** answered that this value was estimated using a well defined quantitative procedure described earlier (see June 2010 meeting). After further discussions on the presence of additional small correlations between some integral values, the participants decided to adopt the correlation data as proposed by JAEA.

5.b) M. Ishikawa reminded the participants about the importance to take into account the analytical modelling errors when analysing the result of the adjustment (see Sg33 November 2010 meeting).

M. Salvatores thanked **M. Ishikawa** for this comprehensive study of the analytical modelling error in deterministic calculations. He suggested circulating a more detailed document to explain the concepts sustaining the proposal as well as the procedure used to estimate the error matrix. He also reminded that the Monte Carlo method should be used as far as possible for the benchmark exercise.

6. Clarification on the use of corrective factors

G. Palmiotti made some clarifications on the use of corrective factors calculated with the ENDF/B-VII library and distributed to all participants. These corrective factors are obtained as a ratio between a very detailed (reference) calculation and a simplified one. Therefore, participants that do not want to fully reanalyze the experiments using their own data library should obtain the calculated integral value by just carrying out the calculation for the simplified model and then multiplying the results by the corresponding corrective factor. It has been shown (see Sg33 November 2010 meeting) that there is a weak dependence of the corrective factors from the library used. **M. Ishikawa** agreed in general but added that corrective factors may actually strongly depend on the library in the case of ZPPR9 sodium voids. **G. Palmiotti** agreed to increase the uncertainty associated with the calculation of ZPPR9 Na voids in order to account for such kind of modelling error (Action 2).

7. WPNCS Expert Group on Uncertainty Analysis for Criticality Safety Assessment

T. Ivanova gave an overview of the progress made in the framework of the WPNCS Expert Group on Uncertainty Analysis for Criticality Safety Assessment (UACSA). As part of the validation approach used in this field, S/U analysis allow assessing the similarity between benchmark experiments and a design system. Then, adjustment techniques are used to assess bias and bias uncertainty in the calculation methods (code+data). As part of a benchmark to assess the whole procedure, the phase III of the UACSA exercise will test techniques and software tools for calculation of k_{eff} sensitivity to neutron cross sections (e.g. 3D vs. RZ models, 1^{st} order perturbation vs. direct calculation).

8. Uncertainty analysis on target systems

8.a) S. Pelloni presented S/U analysis of benchmark experiments and target systems using ERANOS in conjunction with unadjusted libraries (JEFF-3.1/BOLNA, JEF-2.2), as well as with an adjusted library (ERALIB1). The use of the adjusted library significantly reduces the uncertainty but reveals inconsistencies, which certainly support the proposed adjustment exercise.

8.b) R. McKnight presented S/U analysis of FBR and ABR target system multiplication factors. The study was performed with VARI-3D and ERANOS-2.2 codes. Nuclear data from the ENDF/B-VII.0 library were used together with the new COMMARA-2.0 covariance data. The k_{eff} total uncertainty obtained with COMMARA-2.0 data is about 1% for all target systems.

D. Rochman questioned the small uncertainties adopted in COMMARA-2.0 for the high energy region of the ^{241}Pu fission cross-section. **G. Palmiotti** commented that there were long discussions in the US on this issue as shown by the back-and-forth modifications of these values in the successive releases of the AFCI/COMMARA library.

8.c) D. Rochman presented S/U analysis of benchmark experiments and target systems using both the conventional and the Total Monte Carlo (TMC) approach. Sensitivity coefficients to k_{eff} have been calculated with MCNP (except for the ABR cores because of the non-availability of MCNP models at

NRG). Covariance data from TALYS/TENDL have been propagated using these sensitivity coefficients to calculate k_{eff} uncertainties. In some cases, differences in PUFF and NJOY processing were observed in the unresolved resonance region. A few TMC-based uncertainty calculations are still ongoing and final results should be available by the next meeting.

M. Herman and **M. Dunn** inquired about the differences observed between PUFF and NJOY processing. **D. Rochman** proposed to send the TENDL file(s) causing this difference for further investigation.

9. Adjustment exercise – Phase I

9.a) M. Ishikawa presented phase I adjustment results based on JENDL-4.0 data. The integral values were calculated using simplified models and INL corrective factors for all integral parameters (case 0) or for all parameters except ZPPR9 k_{eff} and Na voids, where JAEA as-built Monte-Carlo calculations were performed (case 1). These results show reasonable changes in nuclear data associated with integral C/E values after adjustment within experimental plus analytical modelling uncertainties, except for ZPPR9 Na voids in case 0. Nevertheless, ZPPR9 Na voids results are satisfactory in case 1. The nuclear data contribution to the integral parameter uncertainty is below target accuracy in all cases.

A. Ignatyuk inquired about the change in the ^{239}Pu prompt fission neutron spectrum. **M. Ishikawa** answered that this is a complicated case, but in the end the adjusted spectrum is harder. **M. Chadwick** added that they reached the same conclusion when analysing the spectral index F28/F25 at LANL.
G. Palmiotti wondered about the large C/E discrepancy of 21% observed for ZPPR9 Na void step 3 (central void) in case 0. **M. Ishikawa** explained that part of this discrepancy is due to modelling difficulties, which are accounted for in the analytical modelling error (13% in this specific case). He recommended using case 1 (as-build MC calculations) for ZPPR9 Na voids. **G. Palmiotti** agreed, but noted that benchmark participants should be allowed to use simplified models together with corrective factors. **M. Ishikawa** answered that this option would be fine as long as the analytical modelling error is considered. **G. Palmiotti** will distribute new ZPPR9 corrective factors with increased uncertainties for Na voids (Action 2).

9.b) C. de Saint Jean presented revised adjustment results obtained with preliminary in-house covariance data. Integral parameters and associated sensitivity coefficients to nuclear data have been calculated with the ERANOS/PARIS code and JEFF-3.1.1 data using the new correction factors. A conventional multigroup adjustment was performed in the CONRAD framework. The new correction factors allow improving the chi-square (better C/E values after adjustment) as compared to results shown in November 2010. Further analysis is ongoing to understand the results of the adjustment (e.g. large adjustments of non-sensitive cross-sections with large uncertainties). Final results will include new covariance data as well as nu-bar and Chi uncertainties.

M. Herman commented that a Kalman-based method would prevent any adjustment when there is no sensitivity.

9.c) G. Palmiotti presented adjustment results obtained with the new set of COMMARA-2.0 covariance data. All integral parameters and associated sensitivity coefficients have been calculated with MCNP and ERANOS using ENDF/B-VII.0 data. The most significant nuclear data adjustments are observed for ^{238}U, ^{56}Fe and ^{239}Pu inelastic cross sections, as well as for the ^{235}U and ^{239}Pu capture. All the adjustments on cross sections are within the 1 sigma standard deviation range. The inclusion of integral experiment correlations, at least in this specific case, does not seem to have any significant impact. The uncertainty evaluation performed on target systems shows significant reductions (mostly related to correlations) for k_{eff}, but not as significant for Na voids.

M. Chadwick commented that it is somehow disappointing to see that the uncertainty reduction on integral parameters essentially comes from adjusted correlations. **M. Salvatores** answered that this

benchmark exercise will certainly provide a feedback on cross-section uncertainties and that assessing the reliability of this feedback is also part of the exercise.

9.d) M. Ishikawa presented a simulation of adjustment in a simple case where 3 cross-sections are adjusted on 2 integral data. He demonstrated the effect on the results of variations in cross-section uncertainty, cross-section correlation, sensitivity coefficient and integral data uncertainty.

10. Discussion on next steps

M. Salvatores invited all participants to the meeting to detail their future contributions to Sg33 activities. JAEA (**M. Ishikawa**, K. Sugino) already completed the adjustment benchmark phase I and will wait for the second phase. INL (**G. Palmiotti**), ANL (**R. McKnight**), ORNL (**M. Dunn**, B. Rearden), JSI (**A. Trkov**) and CEA (**C. de Saint Jean**) plan to complete the phase I of the benchmark. **A. Ignatyuk** (IPPE) will discuss possible contributions with G. Manturov. CIAE will contribute when their calculation tools are ready. NRG (**D. Rochman**), PSI (**S. Pelloni**) and KAERI will carry out uncertainty analysis only.

M. Ishikawa proposed an extension to the Sg33 format to store/exchange information on the individual contributions, per isotope and reaction, to the integral data uncertainty. **E. Dupont** and **G. Palmiotti** will circulate new format specifications (Action 3).

M. Salvatores asked all Sg33 members to provide, in Sg33 format, by September 2011, the integral C/E values (and uncertainty if relevant) that they have calculated with their own data library (Action 4). In addition, all participants to the benchmark adjustment exercise should provide, in Sg33 format, by September 2011, the final result of benchmark phase I (Action 4). It is essential for these results to be available in September to allow some comparisons to be performed with the help of the NEA secretariat before the next meeting (Action 5).

The next meeting will be held at the NEA, Issy-les-Moulineaux, France during the week from 28 November to 2 December 2011, in conjunction with JEFF meeting.

11. Actions

1.	E. Dupont All	To compile a list of the most useful references related to S/U methods.
2.	G. Palmiotti	To update ZPPR9 corrective factors taking into account specific modelling difficulties of Na void calculations.
3.	E. Dupont	To circulate format specifications to store isotope/reaction contributions to integral data uncertainty.
4.	All	To complete, by September 2011, the phase I of the benchmark adjustment exercise and distribute the data in the agreed format. All Sg33 members should provide at least the integral C/E values calculated with their own data library.
5.	E. Dupont	To collect input/output data from the phase I benchmark and prepare them for comparison.
6.	E. Dupont	To update the subgroup web page with materials from this meeting and other participant contributions.

Appendix 1

Participants to the 5th meeting of WPEC subgroup 33

NEA, Issy-les-Moulineaux, France

11 May 2011

M. Chadwick	LANL, USA	
M. Dunn	ORNL, USA	
E. Dupont	NEA, OECD	(Secretary)
Z. Ge	CIAE, China	
J. Gulliford	NEA, OECD	
M. Herman	BNL, USA	
A. Ignatyuk	IPPE, Russia	
M. Ishikawa	JAEA, Japan	
T. Ivanova	IRSN, France	
O. Iwamoto	JAEA, Japan	
A. Kahler	LANL, USA	
T. Kawano	LANL, USA	
S.-J. Kim	KAERI, Korea	
R. McKnight	ANL, USA	(Monitor)
G. Palmiotti	INL, USA	(Coordinator)
S. Pelloni	PSI, Switzerland	
A. Plompen	JRC-IRMM, EC	
D. Rochman	NRG, Netherlands	
C. de Saint Jean	CEA, France	
M. Salvatores	INL, USA – CEA, France	(Coordinator)
A. Trkov	IJS, Slovenia	
W. Wang	CIAE, China	
H. Wu	CIAE, China	

Appendix 2

Agenda of the 5th meeting of WPEC subgroup 33

NEA, Issy-les-Moulineaux, France

11 May 2011

9:00 – 9:20 **Introduction**

Welcome, approval of agenda, action items from last meeting. (M. Salvatores)

1. 9:20 – 9:35 **Discussion on Progress of the subgroup actions and release of first deliverable**
(All. M. Salvatores, G. Palmiotti, and E. Dupont drive discussion)

2. 9:35 – 9:55 **Adjustment methodology**

Adjustment methodology in use at CIAE (H. Wu)

3. 9:55 – 10:10 **Experiment analysis**

ZPPR-9 Updated Results (ANL, R. McKnight)

4. 10:20 – 11:00 **Cross section covariance matrix**

Sensitivity/Uncertainty analysis at CIAE (W. Wang)
Release of COMMARA 2.0 to participants (BNL, M. Herman)

5. 11:00 – 11:30 **Experiment covariance matrix**

Discussion and feedback to JAEA proposal (All, M Ishikawa and R. McKnight drive discussion)

6. 11:30 – 11:40 **Clarification on the use of corrective factors** (G. Palmiotti)

7. 11:40 – 12:10 **WPNCS Group on Uncertainty Analyses for Criticality Safety Assessment**

Overview of the progress made at the WPNCS (IRSN, T. Ivanova)

8. 13:30 – 14:30 **Uncertainty evaluation**

Uncertainty analysis with JEFF, ERALIB-1, and BOLNA data (PSI, S. Pelloni)
Uncertainty estimation of target system k_{eff} with COMMARA data (ANL, R. McKnight)
Uncertainty analysis on target systems (NRG, D. Rochman)

9. 14:30 – 16:00 **Adjustment exercise**

Adjustment results based on JENDL-4.0 (JAEA, M. Ishikawa)
Status of CEA Activities in SG33 (C. de Saint Jean)
Preliminary adjustment results based on ENDF/B-VII and COMMARA 2.0 (INL, G. Palmiotti)
Simulation of cross-section adjustment (JAEA, M. Ishikawa)

10. 16:00 – 17:30**Discussion on next steps.**

Next steps, schedule, and next meeting (All)