Summary Record of the 7th 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

22-23 May 2012

The subgroup co-ordinators, **M. Salvatores** and **G. Palmiotti**, opened the meeting and welcomed the participants (see Appendix 1). Apologies for absence were received from I. Kodeli (IJS, Slovenia) and W. Wang (CIAE, China). The proposed agenda was adopted with one more presentation by **C. Perfetti** (ORNL, USA) on benchmark results. The final agenda is available in Appendix 2.

M. Salvatores reviewed the actions from the previous meeting and asked whether IPPE will contribute to the benchmark exercise. **A. Ignatyuk** answered that results should be sent by **G. Manturov**. An updated list of actions is available at the end of this document (see section 6).

1. Plans for COMMARA-3

M. Herman presented plans for the development of COMMARA-3, which will include covariance data for 184 materials associated with ENDF/B-VII.1 data. This new version will contain processed covariance data collapsed into 33 groups using a reactor-like weighting flux (i.e. χ+1/E). It will take into account changes in central values from version VII.0 to VII.1 of the ENDF/B library and will significantly extend covariance information for nu-bar, prompt fission neutron spectra and mu-bar, as well as cross-correlation for a selection of isotopes. The release is expected by the end of FY2013.

M. Salvatores stressed that a beta version of COMMARA-3 prior to the official release is essential for testing purpose. **M. Herman** mentioned that COMMARA-3 is due by September 2013 (i.e. end of FY2013), but a beta release could be available by the end of 2012 already.

2. Review of the results of the benchmark adjustment exercise

S. Pelloni presented revised C/E values and S/U analysis of benchmark experiments. This work was performed at PSI using ERANOS with JEFF-3.1 and ENDF/B-VI.8 evaluated libraries and associated COMMARA-2.0 covariance data. The work on adjustment is ongoing.

S.J. Kim presented an update of S/U analysis performed at KAERI using DANTSYS/SUSD3D codes with JENDL-4.0 and COMMARA-2.0 covariance data. Work is ongoing to develop the code and procedures for cross-section adjustments.

M. Ishikawa commented on the comparison between JENDL-4.0 and COMMARA-2.0 for ^{235}U(n,f) uncertainties in the thermal energy region. He explained that the large uncertainty in JENDL-4.0 was due to a compilation error of the covariance data. An updated ^{235}U evaluation will be made available on the JAEA web site.

H. Wu reported on CNDC progress on nuclear data adjustment and presented revised C/E results and S/U analysis using CENDL-3.1 and JENDL-4.0 data. A modified version of the ZOTT-VL code will be used to adjust cross-sections.

C. Perfetti presented preliminary benchmark results obtained at ORNL using TSUNAMI-1D to calculate sensitivity data files and TSURFER to adjust cross-sections. All calculations were performed using the ENDF/B-VII.0 application library (238 groups) processed at ORNL and SCALE 6.1 covariance data (44 groups).

M. Salvatores and **G. Palmiotti** stressed that the contribution to the benchmark exercise should be as complete as possible and should comply with benchmark specifications (e.g. 33 groups).

G. Aliberti presented results of the benchmark adjustment including fission spectrum and mu-bar in addition to nu-bar and cross-sections. The integral parameters and associated sensitivity coefficients were calculated using the ERANOS code system with ENDF/B-VII.0 data and the adjustment was performed with the GMADJ code using COMMARA-2.0 covariance data.

E. Ivanov mentioned that the use of a direct method to calculate the sensitivity of mu-bar does not properly take into account cross-correlations. **M. Salvatores** noted that the presentation of the χ^2 value before/after adjustment should be homogenised between participants.

T. Ivanova presented preliminary results obtained at IRSN using the SCALE code system and associated ENDF/B-VII.0 application library (238 groups) together with COMMARA-2.0 covariance data (33 groups). The sensitivity profiles were condensed from 238 to 33 groups. The BERING code recently developed at IRSN was used to adjust nuclear data on k_{eff} values. Comparison of these preliminary results with INL data shows significant differences for sensitivity coefficients of ^{238}U and ^{56}Fe (elastic and inelastic) scattering cross-sections and for some C/E values before adjustment. The latter discrepancy might be due to the SCALE group structure, which is not fine enough or not consistent with INL correction factors.

M. Ishikawa commented that the result of the adjustment should not strongly depend on the number of experiments and proposed that another participant also performs the adjustment using only k_{eff} in order to validate this assumption.

D. Rochman presented nuclear data "adjustment" on integral parameters (k_{eff} only) using Monte Carlo (MC) techniques. As for the Total Monte Carlo (TMC) approach, the first steps are to produce thousands of TALYS-based evaluated files using MC sampling of nuclear parameters and to benchmark all files with simulation of integral experiments. The so called Petten method solves the inverse problem of nuclear data adjustment by simply selecting the combination of random files that best reproduce all integral benchmarks. This approach was used to search for the best set of ^{235,238}U, ^{239}Pu evaluations and "adjusted" results were presented for fission, capture, scattering cross-sections and nu-bar.

M. Salvatores commented that there is too much freedom in this approach and that sensitivities could be used to constrain the "adjustment". Moreover, if only the cross sections of three isotopes are considered, some degree of arbitrariness is introduced in the adjustment. **A. Plompen** noted that this method has the advantage to preserve physics since optimal/adjusted nuclear data are calculated using nuclear reaction models.

C. De Saint Jean presented results for the phase I and II of the benchmark exercise with/without adjustment of Chi and nu-bar. Integral calculations were performed with the ERANOS code system, whereas adjustment was made in the Conrad framework using the JEFF-3.1 library and CEA covariance (for phase I) and JENDL, COMMARA covariance (for phase II).

3. Stress tests

G. Palmiotti presented adjustment results obtained after addition of one integral parameter with quite significant initial discrepancy on the C/E value – i.e. C/E ~900 pcm for the k_{eff} of ZPR9-34, which is a ^{235}U core with a reflector in stainless steel (SS). The C/E values obtained after adjustment were satisfactory for all integral parameters and the nuclear data contribution to the uncertainty of ZPR9-34 k_{eff} was reduced by almost a factor 20 thanks to the adjustment of ^{56}Fe and ^{235}U cross-sections and associated covariance data.

M. Ishikawa presented similar results after addition of ZPR9-34 k_{eff} and also a more stringent stress test with adjustment on three additional k_{eff} values from ZPR3-53 (Pu-^{238}U-C core + ^{238}U blanket with C/E ~840 pcm), ZPR3-54 (Pu-^{238}U-C core + Fe reflector with C/E ~1400 pcm) and ZPR6-10 (Pu-C-SS core + SS reflector with C/E ~3400 pcm). It was stressed that although integral C/E after adjustment was excellent in all cases, some changes in the capture cross-sections of ^{239}Pu and ^{56}Fe were beyond nuclear data uncertainties in the case of the most stringent stress test. It was proposed to define criteria to detect the presence of abnormal integral parameters in the adjustment database.

M. Salvatores commented that the nuclear data uncertainties should be checked as well and agreed that there should be a criteria to alert that something is wrong in the integral or differential data in order for further analysis to be performed (e.g. χ^2-test related).

4. Comparison and discussion

E. Dupont reminded the participants that the description of the benchmark input/output format is available on the subgroup web page and presented benchmark results already received (also available on the web page). Software is being developed by the NEA to display and compare benchmark results provided in SG33 format. This software can display sensitivity coefficients and nuclear data with associated uncertainties before/after adjustment, but not covariance data.

G. Palmiotti suggested adding computing capability to make ratio of the results before/after adjustment and also between participants. **M. Salvatores** suggested plotting the uncertainties alone in addition to data and uncertainties. It was suggested to use the NNDC software developed for COMMARA for the comparison of covariance data. After some additional discussions, it was proposed to focus on 10 reactions and to provide feedback to the NEA on what should be compared (action 1).

M. Salvatores presented some ideas on the use of the "a-posteriori" global covariance matrix, which includes correlations between differential and integral parameters. He stressed that this off-diagonal part of the matrix is generally not used and felt this as a loss of information, which might be useful for example to assess the applicability range of the adjusted parameters.

5. Discussion on next steps

G. Palmiotti reviewed the results already available for phase I, II and III of the benchmark exercise. It was agreed to start drafting the final report and to finalise and organise comparison of the results at the same time. Both the draft report and the final results will be reviewed at the next meeting. The new/last deadline to send the results to the NEA is October 2012 (action 2). A comparison of the benchmark results for the 10 most important reactions will be distributed by the end of October 2012 (action 3). **M. Salvatores** proposed an outline and chapter leaders for the final report (see below). Every chapter should be about 3-10 pages long and should be sent to the NEA before the next meeting (action 4).

After some discussions, it was agreed that SG33 should be formally closed in 2013 and that a possible follow up could be a new subgroup involving both reactor physicists and nuclear physicists. The objective would be to interpret the result of the adjustment, especially the adjusted covariance matrix, and to provide useful feedback to improve nuclear data.

The next meeting will be held at the NEA Headquarters, Issy-les-Moulineaux, France on November 29-30, 2012, in conjunction with the JEFF meeting.

Report outline

- Introduction, Scope and Objectives (G. Palmiotti, M. Salvatores)
- Definition of Benchmark steps, rationale and expected results (G. Palmiotti and M. Salvatores)
- Integral experiments: rationale of choice, models, correction factors, etc. Reference systems definition (G. Palmiotti)
- Sensitivity studies and issues (S. Pelloni)
- Covariance data for cross sections. Different sets used and main characteristics (M. Ishikawa)
- Integral experiment uncertainties and correlations (D. McKnight. A report from M. Ishikawa is already available)
- Comparison of integral experiment initial C/E's, uncertainties and reference system uncertainties (G. Palmiotti)
- Adjustment procedures (short reminder of previous deliverable, E. Dupont)
- Adjusted data comparison and analysis. Role of "a-posteriori" covariance matrices. Display of selected results (C. De Saint-Jean)
- Stress tests and their impact (M. Ishikawa)
- Recommendations (All)
- Conclusions (All)

Appendixes

- Teaching example of adjustment methods features (Two group example) (M. Ishikawa)
- Detailed benchmark results (E. Dupont. A CD could be prepared with possible use of NNDC software)

6. Actions

1. All	To send to the NEA, by the end of August 2012, the list of the 10 most important reactions that should be more carefully reviewed when analysing the benchmark results.
2. All	To send to the NEA, by October 2012, in SG33 format, the final results of the benchmark adjustment exercise.
3. E. Dupont	To prepare and distribute, by the end of October 2012, a comparison of benchmark results for the 10 most important reactions.
4. Chapter leaders	To send to the NEA, by mid-November 2012, draft of the chapter(s) under their responsibility.
5. E. Dupont	To update the subgroup web page with materials from this meeting and other participant contributions.

Appendix 1

Participants to the 7th meeting of WPEC subgroup 33

NEA, Issy-les-Moulineaux, France

22-23 May 2012

G. Aliberti	ANL, USA	
Y.-S. Cho	KAERI, Korea	
C. De Saint Jean	CEA, France	
M. Dunn	ORNL, USA	
E. Dupont	NEA, OECD	(Secretary)
T. Fukahori	JAEA, Japan	
Z. Ge	CIAE, China	
M. Herman	BNL, USA	
A. Ignatyuk	IPPE, Russian Federation	
A. Kahler	LANL, USA	
T. Kawano	LANL, USA	
S.J. Kim	KAERI, Korea	
M. Ishikawa	JAEA, Japan	
E. Ivanov	IRSN, France	
T. Ivanova	IRSN, France	
L. Leal	ORNL, USA	
R. McKnight	ANL, USA	(Monitor)
G. Palmiotti	INL, USA	(Coordinator)
S. Pelloni	PSI, Switzerland	
C. Perfetti	ORNL, USA	
A. Plompen	JRC-IRMM, EC	
D. Rochman	NRG, Netherlands	
X. Ruan	CIAE, China	
M. Salvatores	INL, USA – CEA, France	(Coordinator)
H. Wu	CIAE, China	

Appendix 2

Agenda of the 7th meeting of WPEC subgroup 33

NEA, Issy-les-Moulineaux, France

22-23 May 2012

22 May 2012 (start at 13:30)

Welcome and introduction

1. Plans for COMMARA-3 (M. Herman, NNDC)

2. Review of the results of the benchmark adjustment exercise phase I (including uncertainty evaluation). This review includes also some data for phases II and III.

- Revised C/E-values and S/U analysis of benchmark experiments using ERANOS with JEFF-3.1 and ENDF/B-VI.8 evaluated libraries and associated COMMARA-2.0 covariance data (S. Pelloni, PSI)
- Results of Nuclear Data S/U Analysis for Benchmark Exercises Using DANTSYS/SUSD3D with COMMARA-2.0 (S.-J. Kim, KAERI)
- CIAE/CNDC Status report (H. Wu, CIAE)
- Benchmark results (C. Perfetti, ORNL)
- Updated adjustment results (G. Aliberti, ANL)
- Results of the benchmark adjustment exercise (T. Ivanova, IRSN)
- Results of the adjustment exercise (D. Rochman, NRG)

23 May 2012 (start at 8:30)

2. Review of the results (Continued)

- Presentation of (a) Revised adjustment exercise with 3 sets of covariances: COMAC-V0, JENDL-4, COMMARA2; (b) Propagation of uncertainties for both target concepts (C. De Saint Jean, CEA)

3. Stress tests

- Results (G. Palmiotti, INL)
- Results (M. Ishikawa, JAEA)

4. Comparison and discussion

- Status of comparison software at NEA (E. Dupont, all)
  - Cross-sections and associated uncertainties before and after adjustment,
  - C/E and associated uncertainties (data, method, experimental) before and after adjustment (and split by isotope/reaction),
  - Correlation matrices of nuclear data before and after adjustment.
- Understanding/Utilization of « a-posteriori » correlation data (M. Salvatores)

5. Next steps, preparation and content of deliverable, reporting to WPEC