Nuclear Energy Agency

NEA/NSC/WPEC/DOC(2020)20

For Official Use **English text only**

5 November 2020

NUCLEAR ENERGY AGENCY
NUCLEAR SCIENCE COMMITTEE

Working Party on International Nuclear Data Evaluation Co-operation

Meeting of the WPEC Subgroup 47 on the Use of Shielding Integral Benchmark Archive and Database for Nuclear Data Validation

SUMMARY RECORD

12 May 2020
WebEx remote meeting

Dr. Michael Fleming
+33 1 73 21 28 22
michael.fleming@oecd-nea.org

JT03468031

OECD/NEA Nuclear Science Committee

Working Party on International Nuclear Data Evaluation Co-operation (WPEC) Meeting of Subgroup 47 on the Use of Shielding Integral Benchmark Archive and Database for Nuclear Data Validation

WebEx remote meeting

12 May 2020

SUMMARY RECORD

1. Welcome

The Chair, **I. Kodeli**, welcomed the participants (see ***Appendix 1***) and the WPEC Secretariat, **M. Fleming**.

2. Adoption of the agenda

The agenda as described in ***Appendix 2*** was adopted, although the order of the presentations was altered to allow J.-Ch. Sublet to participate and present in the EG-GNDS meeting. The order of the presentations in this record are based on the original agenda.

3. Benchmarking of SuperMC by using different libraries with reactor shielding experiments in SINBAD

B. Li showed work done by the FDS team to validate calculations done with the SuperMC code using SINBAD experiments. Several types of experiments were considered with results shown for neutron spectra and some activation reaction rates. The High Intensity D-T Fusion Neutron Generator (HINEG) facility of INEST was reviewed, which produces a yield of approximately 6.4E12 n/s. This is being used for a range of studies, including neutron leakage experiments and validation of SuperMC, as well as materials irradiation testing, core physics studies and other applications. One example shown was a DFLL tritium breeding module for fusion reactors, which included activation measurements that have been the subject of SuperMC validation work. Results for the VENUS-3 and PROTEUS Core 9 experiments were reviewed, showing generally consistent results with MCNP and the experiments. Other calculations shown included dpa, fast neutron spectra for iron shielding and assessment of ENDF/B-VII.1, ENDF/B-VIII.0, JEFF-3.2 and FENDL-3.1 in several tests.

4. Progress on developmentof additional inputs and CAD models for SINBAD

S. Lilley presented a review of and update on the effort to provide CAD input data and a radiation transport simulation workflow for SINBAD experiments. CAD offers a consistent starting point for any work and can be translated into application-specific geometry descriptions (e.g. CSG). Since many radiation transport code inputs are already available, work was done to test if automatic conversion into CAD was possible for several experiments and, where it was not, CAD was drafted by hand based on the experiment description. These CAD files can then be input into codes such as Fluka, MCNP, PHITS, GEANT, DAG-compatible codes or other codes via meshing. Since the last meeting of SG47, the CSG2CSG code[1], which translates inputs between several codes (including MCNP, MCNP, OpenMC, Serpent, Phits, Fluka) was also used to generate other code inputs. The conversion to CAD occurs through either MCAM/SuperMC[2] or simpleGeo[3], with CAD then imported into ANSYS SpaceClaim[4] and then saved as an ISO 10303-21 Standard for the Exchange of Product model data (STEP) file[5]. A series of checks are performed through volume comparisons (stochastic vs CAD-calculated), 'void' simulations for geometry errors and other code-specific tests. Examples were shown for the IPPE Th ^{252}Cf spheres with STEP file generation and conversion with MCAM/SuperMC and CSG2CSG. Some geometries created were incorrect and testing continues. Another example shown was the ASPIS Fe88 experiment, which has no MCNP input and a CAD geometry was created from schematics. Testing is ongoing with this model, including calculations with unstructured volume meshes and the FETCH2 code[6].

5. KIT contribution to SG-47: progress since June 2019

S. Simakov presented the progress on two actions following the June 2019 meeting of SG47. For the Action 3 item (*provide KFK-1977 gamma measurement data for potential SINBAD evaluation*), the data presented in plots within KFK-2444 (1977) were digitised and later compared with numerical data provided from S.-H. Jiang. These include 3 spheres of 25, 30 and 35 cm diameter. Gamma spectra were compared with the results from IPPE 1985 measurements, showing generally good agreement within the uncertainties. For the Action 4 item (*contribute models for oxygen ORNL broomstick benchmark and 91.44 cm liquid oxygen data if of sufficient quality for SINBAD*), it was noted that the authors used an analytic expression to compute the uncollided neutron spectrum[7] and this may partially justify the absence of the model input. An MCNP model was generated from three publications[8], however the neutron transmission spectra for the 24 and 36 inch oxygen samples are not in the SINBAD database. These would be of interest if ORNL or another

1 Available at https://github.com/makeclean/csg2csg

2 See https://doi.org/10.1016/j.anucene.2014.08.058

3 Available for download from: https://theis.web.cern.ch/simplegeo/

4 See https://www.ansys.com/products/3d-design/ansys-spaceclaim

5 See https://www.iso.org/standard/63141.html

6 See http://www.imperial.ac.uk/earth-science/research/research-groups/amcg/software/fetch/

7 See ORNL-TM-2242

8 NSE 27 299 (1967), ORNL-TM-2242 (1968) and ORNL-TM-3868 (1972)

organisation could provide the data. The results from calculations with the Monte Carlo model confirmed that the analytic approximation was reasonably accurate, but the full simulation capabilities now offered allow analysis of topics such as the impact of detector resolution and the calculation of sensitivities to nuclear data. Testing the ENDF/B-VII.1 (adopted in JEFF-3.3) and ENDF/B-VIII.0 data for ^{16}O shows better agreement with the previous version, although further study is required.

6. UKAEA experience and involvement with SINBAD

A. Valentine gave an overview of the UKAEA work related to SINBAD, describing the Applied Radiation Technology (ART) group its activities UKAEA programme of work. This includes development of the FISPACT-II inventory code[9]. Recent work with SINBAD has included cross-verification with different codes, including Serpent 2[10] and the most recent version of MCNP. Calculations for the FNG HCPB mock up experiment were shown with results for tritium activity for various lithium carbonate pellets. Results were also shown for simplified demonstration fusion power plant blanket modules, with comparisons in nuclear heating shown. This identified serious discrepancies due to negative cross sections in the JEFF-3.3 ACE data that was being used. Serpent 2 flagged this as an error while MCNP ignored this issue. A check on the FENDL-3.1d ACE files found that 9 DPA or heating values were negative in the library.

Work is continuing with the testing of newly added variance reduction techniques in Serpent 2 and the creation of additional experimental and computational benchmarks to test the code, including for so-called ‘rigorous 2-step’ shut-down dose calculations. Several comments were made regarding SINBAD:

- Several input decks are not valid and cannot be run without modifications – they also lack comments or other description inside the files
- Documentation is often provided from publications and not based on a standardised evaluation format (as with ICSBEP, for example)
- More information on the calculation model would be appreciated
- Benchmarks require NEA and/or RSICC requests, which is inconvenient
- There is little photon/photonuclear experimental data
- Neutron and photon heating benchmarks are of interest to the fusion community
- Addition of other code inputs would be welcome for SINBAD
- Several older benchmarks have no MCNP input

In discussion, it was noted that more content for SINBAD (e.g. updates to or new model inputs, documentation or more experiments) would be very welcome. The committee responsible for SINBAD is responsible for reviewing any potential additions but within the WPEC SG47 new inputs and data are already being provided and these will be submitted for inclusion in SINBAD officially.

[9] See https://doi.org/10.1016/j.nds.2017.01.002

[10] See http://montecarlo.vtt.fi/ for more information

With the new £220 million Spherical Tokamak for Energy Production (STEP) programme at UKAEA, shielding benchmarks for fusion applications will be an essential activity. New experiments include studies of oxygen activation in cooling water and a WCLL neutronics mock-up being carried out at ENEA/FNG.

7. Update of SINBAD status and reminder of SG47 objectives

I. Kodeli began with some memories of Massimo Salvatores, who passed away in March. Massimo was a leader in the shielding benchmark work of the 1980s and 1990s, Chairing the NEACRP Shielding Benchmark Group. He reminded the participants of the scope and objectives of the group, which aims to improve the use of SINBAD in nuclear data validation. Recent news regarding SINBAD includes the continuation of a quality review by A. Milocco on a range of experiments from JANUS, ASPIS and PCA Replica. SuperMC inputs are being contributed for a range of SINBAD experiments, as well as TORT inputs for ASPIS Fe88 and PCA Replica. The October 2019 TRG meetings reviewed two new Frascati measurements and HIMAC, with work continuing. Weight windows and other variance reduction tools are being integrated for inputs, sensitivity profiles are being calculated for select experiments and CAD geometries are being provided in STEP or other formats. The current set of experiments includes 102 entries with 18 provided by RSICC, covering reactor shielding and dosimetry (48), fusion neutronics (31) and accelerator shielding (23). The FNG copper, ASPIS-Fe88 and TIARA Fe/concrete[11] experiments were reviewed. A new sinbadAspis tool has been created by A. Milocco to generate MCNP benchmark models using the open-source CombLayer code[12]. This code is available on request for testing. Transport code inter-comparison studies have been started with codes including MCNP, ADVANTG, Serpent (2), TRIPOLI, Geant4, DORT, TORT, FLUKA, PHITS, MARS and MCBEND. Several potential future SINBAD evaluations were discussed, ranging from the LLNL spheres (where work is already planned) to new potential entries from Chinese laboratories, additional cases from existing entries and fusion D-T experiments. Since the SG47 kick-off, new SuperMC inputs have obtained, reviews for several experiments have been carried out (FNG Cu, ASPIS Fe88, REPLICA, IPPE Fe) and CAD geometries are being included for experiments. A SINBAD review group has held in 2019 and re-evaluations will be included in an updated database.

8. Compilation of Nuclear Data Experiments for Radiation Characterisation – CoNDERC – to serve SG-47

J.-Ch. Sublet provided an overview of the recently launched Compilation of Nuclear Data Experiments for Radiation Characterisation (CoNDERC). The overarching objective is to transfer experimental integral radiation information into robust digital technology for the purposes of verification and validation. This aims to be very broad in application, including radiation transport, time-dependent calculations, spectral indices/reaction rates, and other data. Work with spectra, spectral indices/reaction rates, integral indices and fusion events is already done while more work in fission events and integro-differential data is ongoing. New initiatives related to ASPIS and TIARA have been recently started. A review of

[11] Including notes from https://www-nds.iaea.org/publications/indc/indc-nds-0785/

[12] Available online at: https://github.com/SAnsell/CombLayer

ICSBEP, IRPhE and the IAEA TRS 480[13] is being carried out to identify reaction rates of interest and provide MCNP input decks with physics cards that allow converged results (which are typically much more computationally challenging than integral quantities such as k_{eff}). Fusion decay heat from the JAEA FNS experiments were reviewed, as well as the work to create an integral cross section database drawing upon the *Atlas*, *Handbook of Chemistry and Physics*, KADoNiS and data in the UKAEA-R(15)30 report[14].

9. Interpretation of the ASPIS and JANUS shielding experiments

G. Rimpault presented work done on the ASPIS Fe88 and JANUS Phase 2 and 7 experiments using TRIPOLI-4 and different JEFF nuclear data libraries with permutations of selected isotopes to which the system is generally sensitive. These experiments were carried out in the 1980s and 1990s in an experimental zone installed behind graphite reflectors of the NESTOR reactor in Winfrith, UK. In this zone, a HEU aluminium alloy fission plate was subjected to neutrons from the reactor. A shielding zone was placed next to the fission plate, composed of various materials with activation detectors sandwiched between layers. ASPIS Fe88 and the JANUS Phase 2 and 7 experiments included mixtures of mild and stainless steels, sodium and boron carbide. Gold capture below the cadmium barrier and the threshold $^{32}S(n,p)$ were used with IRDFF-1.05 and EAF-2010 used for the activation calculation. Trends as a function of shielding depth for the gold measurements were broadly in agreement for the ASPIS Fe88 but under/over-estimation trends increase to a bias of approximately 40% in mild steel, depending on the ^{56}Fe evaluation used. This depends not only on cross sections but the scattering angular distributions. The JANUS phase 2 experiments include layers of stainless steel and sodium and show a gold capture bias in all libraries within the stainless steel layer. The sulphur reaction shows bias trends in the steels that are further complicated in the sodium layer. The phase 7 experiment replaces stainless steel with boron carbide and here the sodium measurements show good agreement for gold following any bias that was introduced in the steel and/or B_4C layers. These trends require sensitivity calculations to identify the responsible reaction data.

10. Quantifying the indicators of the ageing under irradiation

M. Brovchenko presented the perspective of the IRSN as a TSO that must provide technical opinions on the ageing of materials in nuclear reactors. Having precise and validated tools is essential for this activity and work has been done to perform code to code comparisons as well as benchmarking against experiments. Calculations are typically performed in two phases, with a reactor core calculation generating boundary source terms that are used in Monte Carlo shielding calculations (e.g. outside the RPV). Results using the MCNP Weight Window Generator (WWG), ADVANTG and MCNP-based Direct Statistical Approach (DSA) can generate significantly different results and these need to be better understood and benchmarked. DPA calculations are of great interest and methods including NRT, DART and MCNP with SRIM have been tested. Results vary by up to a factor of four with nearly universal under prediction using the simply mono-atomic NRT as generated by NJOY. Studies such as the VENUS-1 and VENUS-3 benchmarks[15] are

[13] STI/DOC/010/480 ISBN 978-92-0-151714-2

[14] Available at https://fispact.ukaea.uk/documentation-2/reports/

[15] See https://www.oecd-nea.org/science/docs/2000/nsc-doc2000-5.pdf

crucial for establishing the validation case and these also provide feedback for the re-evaluation of nuclear data to meet the needs of users.

11. Validation of computer code TORT using RC Řež Iron Spherical Assemblies producing neutron and gamma mixed fields

B. Jansky presented work done with the TORT code and BUGLE-7/96 libraries for the Řež iron spherical assemblies. Leakage neutron and gamma spectra were compared with the 20, 30, 40, 50 and 100 cm diameter sphere with a ^{252}Cf source. TORT was used with S8 P3 calculations and BUGLE data derived from the ENDF/B-VI and VII libraries. Once renormalised, averaged spectra over a multi-group structure were compared with some agreement found for specific energy ranges, although results were varied. Gamma spectra showed even more variation.

12. Using LLNL Pulsed Spheres for Nuclear Data Validation

D. Neudecker presented work done to determine which nuclear data observables may be validated with the 75 LLNL pulsed-sphere neutron-leakage spectra for 20 different materials. A set of MCNP inputs[16] were run with ENDF/B-VII.1 and ENDF/B-VIII.0 data and a set of sensitivity profiles were generated for 17 spheres where C/E values were not ideal. ^{6}Li, ^{12}C, ^{16}O, ^{24,25}Mg, ^{27}Al, ^{48}Ti and $^{206\text{-}208}$Pb all showed significant disagreement between the calculated and experimental spectra. Comparisons between the C/E and sensitivity profiles indicate that light elements are generally sensitive to elastic and inelastic scattering cross sections (particularly MT=51) and the angular distributions of these channels. In specific cases the results were sensitive to the inelastic continuum double-differential data. Actinide cases are highly sensitive to the fission cross section, neutron energy distribution and the average neutrons per fission.

13. Next meeting and any other business

The next meeting will be held during the week of WPEC meetings in May 2020, although earlier meetings may be arranged, as required. Actions agreed at this meeting and the summary of updates for previous actions are summarised in ***Appendix 3***.

[16] See LA-UR-05-0879

APPENDIX 1

List of registrants to the 12 May 2020 Meeting of Subgroup 47 on Use of Shielding Integral Benchmark Archive and Database for Nuclear Data Validation

WebEx Meeting

	Name	Surname	Representing	Notes
1	John	BESS	UNITED STATES	
2	Doug	BOWEN	UNITED STATES	
3	Mariya	BROVCHENKO	FRANCE	
4	Oscar	CABELLOS	SPAIN	Co-chair
5	Yurdunaz	CELIK	BELGIUM	
6	Theresa	CUTLER	UNITED STATES	
7	Yaron	DANON	UNITED STATES	
8	Marie-Anne	DESCALLE	UNITED STATES	
9	Yanyan	DING	CHINA	
10	Michael	FLEMING	NEA	Secretariat
11	Mark	GILBERT	UNITED KINGDOM	
12	Joetta	GODA	UNITED STATES	
13	Wim	HAECK	UNITED STATES	
14	David	HAYES	UNITED STATES	
15	Jesse	HOLMES	UNITED STATES	
16	Jesson	HUTCHINSON	UNITED STATES	
17	Raphaelle	ICHOU	FRANCE	
18	Bohumil	JANSKY	CZECH REPUBLIC	
19	Albert	KAHLER	UNITED STATES	
20	Soon Sam	KIM	UNITED STATES	
21	Ivan-Alexander	KODELI	SLOVENIA	Chair
22	Bor	KOS	SLOVENIA	
23	Luiz	LEAL	FRANCE	Co-chair
24	Dieter	LEICHTLE	GERMANY	
25	Amanda	LEWIS	UNITED STATES	
26	Emily	LEWIS	UNITED KINGDOM	
27	Bin	LI	CHINA	
28	Steve	LILLEY	UNITED KINGDOM	
29	Julie-Fiona	MARTIN	NEA	
30	Alberto	MILOCCO	ITALY	
31	Benjamin	MURPHY	UNITED STATES	

32	Denise	NEUDECKER	UNITED STATES	
33	Gustavo	NOBRE	UNITED STATES	
34	Lee	PACKER	UNITED KINGDOM	
35	Chris	PERFETTI	UNITED STATES	
36	Arjan	PLOMPEN	BELGIUM	
37	Gerald	RIMPAULT	FRANCE	
38	Evgeny	ROZHIKHIN	RUSSIA	
39	Georg	SCHNABEL	AUSTRIA	
40	Stanislav	SIMAKOV	GERMANY	
41	Alejandro	SONZOGNI	UNITED STATES	
42	Jean-Christophe	SUBLET	IAEA	
43	Kenichi	TADA	JAPAN	
44	Nicholas	THOMPSON	UNITED STATES	
45	Andrej	TRKOV	SLOVENIA	
46	Alex	VALENTINE	UNITED KINGDOM	
47	Olga	VILKHIVSKAYA	UNITED KINGDOM	
48	Haicheng	WU	CHINA	
49	Michael	ZERKLE	UNITED STATES	
50	Gasper	ZEROVNIK	BELGIUM	

APPENDIX 2

OECD/NEA Nuclear Science Committee

Working Party on International Nuclear Data Evaluation Co-operation (WPEC)Meeting of Subgroup 47 on Use of Shielding Integral Benchmark Archive and Database for Nuclear Data Validation

WebEx Meeting, 12 May 2020

AGENDA

Duration	PDT (CA, USA)	CEST (Paris)	JST (Tokyo)	Topic	
00:10	02:00	**11:00**	18:00	Welcome	I. Kodeli
00:10	02:10	**11:10**	18:10	Review of actions	I. Kodeli
00:20	02:20	**11:20**	18:20	Analysis of validation results from the IPPE iron sphere benchmark	H. Wu
00:20	02:40	**11:40**	18:40	Progress on development of additional inputs and CAD models for SINBAD	S. Lilley
00:20	03:00	**12:00**	19:00	KIT contribution to SG-47: progress since June 2019	S. Simakov
00:20	03:20	**12:20**	19:20	UKAEA experience and involvement with SINBAD	A. Valentine
00:20	03:40	**12:40**	19:40	Update of SINBAD status and reminder of SG47 objectives	I. Kodeli
00:20	04:00	**13:00**	20:00	Short break	
00:20	04:20	**13:20**	20:20	Compilation of Nuclear Data Experiments for Radiation Characterisation - CoNDERC	J-Ch. Sublet
00:20	04:40	**13:40**	20:40	Interpretation of the ASPIS and JANUS shielding experiments	G. Rimpault
00:20	05:00	**14:00**	21:00	Quantifying the indicators of the ageing under irradiation	M. Brovchenko
00:20	05:20	**14:20**	21:20	Validation of computer code TORT using RC Rez Iron Spherical Assemblies producing neutron and gamma mixed fields	B. Jansky
00:20	05:40	**14:40**	21:40	Using LLNL Pulsed Spheres for Nuclear Data Validation	D. Neudecker
00:45	06:00	**15:00**	22:00	Discussion	
	06:45	**15:45**	22:45	Close	

APPENDIX 3

OECD/NEA Nuclear Science Committee

Working Party on International Nuclear Data Evaluation Co-operation (WPEC)Meeting of Subgroup 47 on Use of Shielding Integral Benchmark Archive and Database for Nuclear Data Validation

Actions agreed at the 12 May 2020 Meeting of Subgroup 47 on the Use of Shielding Integral Benchmark Archive and Database for Nuclear Data Validation

1. (**Bin Li**, FDS): potential FDS shielding benchmarks to be considered for SINBAD, e.g. DFLL TBM (ASAP)
2. 2. (**S. Simakov**, KIT): Provide KFK-1977 gamma measurement data for potential SINBAD evaluation
3. (**S. Simakov**, KIT): Contribute models for Oxygen ORNL broomstick benchmark and 91.44 cm liquid O data if of interest (sufficient quality) for SINBAD
4. (TBD, **ORNL**): investigate the availability of Broomstick experimental data for 24” and 36” O spheres.
5. (**A. Valentine, CCFE, G. Rimpault,** CEA, All): Contribute Serpent, TRIPOLI and other computer code input data of shielding benchmarks to WPEC SG47 and/or IAEA repository (2021 meeting).
6. (**D. Neudecker,** LANL, **O. Cabellos**, UPM): Contribute sensitivities for LLNL benchmarks to WPEC SG47 (2021 meeting).
7. (**S. Lilley -** UKRI STFC**, I. Kodeli**) Provide CAD geometry for IPPE, FNS, FNG, ASPIS and ISIS benchmarks
8. (**B. Jansky**, CVREZ) Contribute TORT & MCNP input data of Rez Fe sphere and slab benchmarks to WPEC SG47 and/or IAEA repositories (ASAP)
9. (**M. Fleming**, NEA) Follow up with the revision of SINBAD benchmarks (e.g. ASPIS)

Status of actions agreed at the 24 June 2019 Meeting of Subgroup 47 on the Use of Shielding Integral Benchmark Archive and Database for Nuclear Data Validation

1. (**G. Lomakov**, IPPE): Provide comments and review of the FNG Cu benchmark evaluation (beginning 2020) DONE
2. (**G. Lomakov**, IPPE): Provide information on the Neutron transmission experiments (1960th) to be included in SINBAD (next meeting)
3. (**S. Simakov**, KIT): Provide KFK-1977 gamma measurement data for potential SINBAD evaluation Reported at 32nd WPEC meeting (ongoing)
4. (**S. Simakov**, KIT): Contribute models for Oxygen ORNL broomstick benchmark and 91.44 cm liquid O data if of interest (sufficient quality) for SINBAD Reported at 32nd WPEC meeting (ongoing)
5. (**Simakov, Kodeli, Milocco**): resolve the issue of dividing by cosine for FNS-O Still ongoing
6. (**Y-K. Lee**, CEA): Contribute TRIPOLI input data of few SINBAD benchmarks to WPEC SG47 (2020 meeting)
7. (**Y.-K. Lee**, CEA): Present a description of the Mn bath experiment for potential inclusion in SINBAD (2020 meeting)
8. (**S. Lilley** - UKRI STFC**, I. Kodeli**) Provide CAD geometry for IPPE, FNS, FNG, ASPIS and ISIS benchmarks Reported at 32nd WPEC meeting (ongoing)
9. (**Jun Zou**, FDS): Provide SuperMC inputs for the set of SINBAD benchmarks (e.g. OKTAVIAN, FNS, FNG, IPPE, Kant) (beginning 2020) DONE
10. (**J. Zou**, FDS): Proposals of potential FDS shielding benchmarks to be included in SINBAD, such as HINEG (2020 WPEC meeting)
11. (**H. Wu**, CIAE) Contribute 14 MeV Fe benchmark data to SINBAD (ASAP)
12. (**B. Jansky**, CVREZ) Contribute Rez Fe sphere and slab benchmark data to SINBAD (ASAP) Rez Fe sphere submitted for review at 2020 ICSBEP TRG
13. (**C. Murphy**, Winfrith) Investigate the possible release of ASPIS benchmark data which are not yet in SINBAD (ASAP)
14. (**O. Cabellos**, UPM) Provide MCNP models and sensitivity profiles for LLNL, FNS, Oktavian benchmarks DONE (Oktavian & FNS)
15. (**I. Kodeli**, IJS) Provide updated SINBAD data for ASPIS Fe88 benchmarks Ongoing