Nuclear Energy Agency

NEA/NSC/WPEC/DOC(2020)19

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 45 Validation of Nuclear Data Libraries (VaNDaL) Project

SUMMARY RECORD

11 May 2020
WebEx remote meeting

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

JT03468027

OECD/NEA Nuclear Science Committee

Working Party on International Nuclear Data Evaluation Co-operation (WPEC)
Meeting of Subgroup 45 Validation of Nuclear Data Libraries (VaNDaL) Project

WebEx remote meeting

11 May 2020

SUMMARY RECORD

1. Welcome

The Chair, **W. Haeck**, who took over the leadership of this subgroup at the request of the original co-ordinator, **M. White**, 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 without modification.

3. OECD/NEA WPEC SG45 progress review

W. Haeck opened the meeting with a review of the status of the subgroup, summarising the status of the contributed input files, cross-comparisons, the input file QA document, calculation results and material balance tables. The NEA GitLab has a WPEC SG45 working area that contains contributions from three organisations:

- IAEA-NDS (MCNP)[1]: A set of ~2800 total cases based on the Skip Kahler suite with additional sources including the ICSBEP CD inputs or inputs taken from the PDF input copies. Some inputs have been generated directly by IAEA but all have been verified and in many cases include format or other corrections. There are several tallies for spectra or other quantities beyond k_{eff}.
- NRG (MCNP)[2]: A large set of ICSBEP benchmarks that draw upon the ICSBEP CD and PDF inputs with various corrections. More than 300 inputs were generated directly by NRG in the past. This suite also bas IRPhE, β_{eff} and Rossi-α

[1] Stored privately for SG45 work at: https://git.oecd-nea.org/science/wpec/sg45/contrib/iaea-nds

[2] Stored privately for SG45 work at: https://git.oecd-nea.org/science/wpec/sg45/contrib/nrg

benchmarks that have wider application[3]. It has been routinely used in testing major library evaluations. This suite is described further in ***Section 6***.

- JAEA (MVP)[4]: A set of ~770 ICSBEP inputs for the Japanese MVP Monte-Carlo code that have been used in verification and validation of JENDL data. This is an excellent source of information that, in comparison to the other suites, has been independently generated and offers an excellent cross-comparison opportunity.

Additional contributions from LANL, LLNL and ORNL may be made available and could include other codes. LANL is preparing a new meta-suite that incorporates inputs from WHISPER, the LANL NCS suite, the XCP-5 Nuclear Data Team suite and inputs from NRG. The release process for this is still ongoing.

The inter-comparison study between DOE NCSP and IRSN resulted in several findings. LANL has reviewed 18 HEU and 10 Pu experiments as a result and found inconsistencies that will be put into the SG45 report. Some 70 cases were reviewed by LANL and 33 input files revised, with several changes resulting in over 500 pcm difference. Typically, these are due to geometry modifications, although materials can play a significant role. HMF-077 was removed due to feedback from LLNL. Some nomenclature issues remain, including differences in how simple/detailed models, impurities, revision numbers and natural abundancies are addressed.

Following the previous meeting, it was agreed that the blocking issue for creating a VaNDaL suite is a common QA document where the basic procedures and organisation will be agreed. This is being prepared with N. Leclaire leading and will stored/developed in the NEA GitLab[5].

A calculation exchange format has been formalised in a JSON schema and is documented in the LANL report LA-UR-19-32580. This information will also be included in the SG45 report on the NEA GitLab although release of the LaTeX source has been delayed. Material balance tables can also be stored in this schema and a description of this is being drafted. This will provide a straight-forward and easily serialised structure that can be populated by different contributors and the DICE database. Work is already ongoing at LANL to generate data manually for these tables.

4. Procedure for Creating, Reviewing, and Submitting Input Files into the Benchmark Library

N. Leclaire presented the process that is being established for the benchmark input library that is being created by SG45. The objective is to standardise the input file creation, review and maintenance, with a standardised procedure and some description for how to use the benchmarks in calculation/validation work. This relies heavily on the work by LANL and IRSN shown at previous SG45 meetings.

The general process should of course begin with a review of the benchmark description, creation of a benchmark model (often simplified to some extent) and input file, verification of the input files and results from simulation, archiving of the input file and documentation

[3] See, for example, https://doi.org/10.13182/NSE03-107

[4] Stored privately for SG45 work at: https://git.oecd-nea.org/science/wpec/sg45/contrib/jaea-mvp

[5] Available to SG45 participants here: https://git.oecd-nea.org/science/wpec/sg45/documents

of the benchmark results. For the benchmark review, section 3 of the ICSBEP documentation is the primary focus and section 1 is used where additional information/clarification is required. Any inconsistency should be clarified (e.g. with the code inputs in the ICSBEP) and reports should be sent to the NEA, ICSBEP co-ordinator and benchmark author. For the inputs themselves, inputs should follow the ICSBEP evaluation and case number should be taken form section 3 of the specifications (e.g. heu-met-fast-001). Where no case number is given (e.g. a unique benchmark), the case number is 001. Where two or more models (detailed/simplified) are provided, these should be reflected in the input file name. The ICSBEP revision number should always be referenced, with a revision 0 as default. Optionally for a suite with multiple code inputs, the code itself could optionally be labelled within the input file name or within a database/folder structure. Material specifications should come from section 3 of the benchmark exactly as described. All TSL data should be clearly indicated and natural isotopes should be specified if no decomposition is provided. If/when isotopes are not available, a simple substitution scheme is required (e.g. carbon isotopes as a 'natural' evaluation), but this will be determined on a case-by-case basis. Geometry is code-specific (e.g. CSG for codes like MCNP with the provided surfaces) and should be identical to the handbook at 4 decimal places.

The review of input files is mandatory and forms the basis of the value of the SG45 output. Organisations involved in this work have very well-defined processes and cross-comparison of the techniques used in participating organisations will be used to populate the SG45 document describing common QA processes. All input files, balance files and other associated documentation will be included in a version-controlled git repository, with directory/subdirectory structure identifying the benchmark and case. Revisions and multiple model types will be designated by the filename. Comparison of the verification and validation methods is ongoing and will be included in the SG45 report. It was proposed to include calculation tools used (including version numbers), lists of experimental values and any calculated values (for all codes) with comparisons, comments on any deviations from the benchmark specifications and analysis of C/E differences, where applicable.

5. Policy driven input file generation applied to MCNP

W. Haeck presented a proposal for a 'policy-driven' approach for input file generation and use, based on the experiences at LANL where multiple different inputs had been developed and used for the same benchmark with non-negligible differences using the same code. The general strategy is to have a template input for specific codes that does not rely on choices such as nuclear data libraries, isotopics, etc. An input pre-processor will take a specific nuclear data organisation input (e.g. 'xsdir') and set of user policies to generate code-compliant inputs. A set of policy areas were identified and will be included in the SG45 report, including policies on abundance data, missing data files or isotopes, etc. Header information is suggested to keep track of these choices and an example was shown.

Work on a new Python MCNP input parser is ongoing. The tool currently can interpret inputs and perform modifications to materials (e.g. change isotopes/natural and atom densities) and change physics options, as well as write the modified file contents to a new input. Example template and generated MCNP files were shown for PMF-001 where the header policy information, physics options and material modifications were applied in this 'policy-driven' way in the pre-processing.

6. NRG contribution to the SG45 repository

S. van der Marck discussed the NRG suite that is now included in the NEA GitLab, as discussed in ***Section 3***. The suite contains several inputs for ICSBEP and IRPhE experiments. For ICSBEP, 832 compound, 570 metal, 1060 solution and 82 miscellaneous benchmarks are included with the material and spectra broken down in the presentation. Other benchmarks include JOYO-LMFR-RESR-001, RCA-LWR-EXP-001 and other β_{eff} and Rossi-α experiments, including experiments from FCA, Mascura, SHE, Sheba, SNEAK, IPEN/MB-01, TCA, Winco slab tanks, ZRP/ZPPR and other LANL cases. The suite is provided with a 'job' shell script that generates MCNP inputs with a set of parametrised options, including nuclide names, abundances and nuclide masses. There is also a file that sets these for the user as an example. This script generates 'inp' files in each directory that can then be executed with MCNP. While the suite contains a large number of inputs, only 314 of the cases have been created at NRG and these were made approximately 15 years ago, based on the ICSBEP edition of that time. No recent verification of the consistency with updated ICSBEP evaluations has been made. The other inputs were based on the ICSBEP DVD inputs, with some corrections made and reported. Notably, several older inputs have omitted or replaced elements that are not consistent with the benchmark.

7. Development of software to automate the computational analyses of fusion relevant benchmarks

S. Simakov presented a systematic and automatic approach to nuclear data validation using spectral response (energy array) benchmarks. This procedure occurs through a sequence of: (1) modification/generation of MCNP input for an experiment; (2) MCNP simulation with tally recordings; (3) processing of MCNP output file; (4) comparison with experimental data and (5) calculation of statistical test parameters (e.g. 'chi-squared'). This was demonstrated with the IPPE iron shell ^{252}Cf spontaneous fission experiments in ICSBEP. The IPPE experiments cover the largest secondary neutron energy range, but were also compared with similar experiments performed at KFK (1977) and NIST (2000). The original MCNP was modified with updated libraries, isotopic carbon and update to the Mannhart Standard for PFNS and ENDF/B-VII.1 for DFNS. The calculation scheme involves shell scripts that modify files with sed and execute fortran programs that parse tally files and calculate the required quantities. With this example, the 5 to 750 keV 50 cm sphere chi-squared value was calculated for ENDF/B-VIII.0 and JEFF-3.3, giving 2.76 and 4.18, respectively. Future work will focus on further modifications to the inputs to address the two tallies that correspond to two physical detectors, extension of this procedure to all six IPPE spheres and inclusion of gamma leakage spectra.

8. Analysis of ICSBEP U233-SOL Benchmarks

Motivated by the strong trends in above-thermal fission fraction (ATFF) in ^{233}U solution benchmarks shown in the ENDF/B-VIII.0 testing, **A. Trkov** showed a set of analyses that focused on the impact of ^{233}U PFNS and thermal constants. Permutations from the ENDF/B-VIII.0 included (1) updated ^{233}U PFNS; (2) updated ^{233}U PFNS and thermal constants and (3) updated ^{233}U PFNS and thermal constants and replaced ^{16}O with that from ENDF/B-VII.1. A collection of ^{233}U solution benchmarks including UST002-004, 006-007 and 010-017, were tested and graphs were shown of k_{eff} deviations as a function of the fraction of epithermal fissions (similar to ATFF). A clear decreasing trend with increasing above-thermal fission fraction was shown and this decreased with the various changed proposed. Breaking these down by individual benchmarks showed significant trends in UST-015 (Falstaff II), for example, although some cases (e.g. UST-014 PNL 'array of bottles') may require more attention in the models and interpretation of the results before more robust conclusions may be drawn.

9. OECD/NEA WPEC SG45: The way forward

W. Haeck discussed the next steps for the SG45 project, focusing on the contribution from LANL. A subset of the Whisper suite already under the LANL QA process will be archived in the format described ***Section 5***, with verification against material balance tables. Header information will be provided in a standardised format. As the pre-processing tools may or may not be made public under the LA-UR process, the procedurally-generated inputs may be provided alone. This will be extended to include Pu, HEU, IEU, LEU and U233 systems, in time, and complemented with the original NRG suite entries. Other code inputs can be added in parallel or after the MCNP contribution – ideally with sufficient time to resolve any outstanding issues in cross comparison using the common output schema discussed in ***Section 3***. Since mass balance tables are required in this QA process, any additional tables would be very valuable. In discussion, it was remarked that the NEA has already made many such tables available via the DICE tool. This is summarised in the 'Balance Tables in the IKCSBEP Handbook', presented by E. Rozhikhin, at the June 2019 meeting of SG45.

10. Next meeting and any other business

The subgroup is nearing its final meeting in 2021, although with the delays caused by Covid-19 there may be scope for extensions at the discretion of the WPEC. To keep up the progress another meeting will be held via WebEx in November, alongside other WPEC meetings.

APPENDIX 1

List of registrants to the 11 May 2020 Meeting of Subgroup 45 Validation of Nuclear Data Libraries (VaNDaL) Project

WebEx Meeting

11 May 2020

	Name	Surname	Representing	Notes
1	Jennifer	ALWIN	UNITED STATES	
2	Bret	BECK	UNITED STATES	
3	David	BERNARD	FRANCE	Co-chair
4	John	BESS	UNITED STATES	
5	Doug	BOWEN	UNITED STATES	
6	Oscar	CABELLOS	SPAIN	
7	Roberto	CAPOTE	IAEA	
8	Yurdunaz	CELIK	BELGIUM	
9	Jeremy	CONLIN	UNITED STATES	
10	Mark	CORNOCK	UNITED KINGDOM	
11	Theresa	CUTLER	UNITED STATES	
12	Yaron	DANON	UNITED STATES	
13	Marie-Anne	DESCALLE	UNITED STATES	
14	Isabelle	DUHAMEL	FRANCE	
15	Michael	FLEMING	NEA	Secretariat
16	Daniela	FOLIGNO	NEA	
17	Tim	GAINES	UNITED KINGDOM	
18	Godfree	GERT	UNITED STATES	
19	Mark	GILBERT	UNITED KINGDOM	
20	Wim	HAECK	UNITED STATES	Co-chair
21	Michal	HERMAN	UNITED STATES	
22	Andrew	HOLCOMB	UNITED STATES	
23	Jesson	HUTCHINSON	UNITED STATES	
24	Raphaelle	ICHOU	FRANCE	
25	Evgeny	IVANOV	FRANCE	
26	Albert	KAHLER	UNITED STATES	
27	Ivan-Alexander	KODELI	SLOVENIA	
28	Stefan	KOPECKY	BELGIUM	
29	Luiz Carlos	LEAL	FRANCE	

30	Nicolas	LECLAIRE	FRANCE	
31	Amanda	LEWIS	UNITED STATES	
32	Fausto	MALVAGI	FRANCE	
33	Julie-Fiona	MARTIN	NEA	
34	Caleb	MATTOON	UNITED STATES	
35	Jordan	MCDONNELL	UNITED STATES	
36	George	MCKENZIE	UNITED STATES	
37	Franco	MICHEL-SENDIS	FRANCE	
38	Gustavo	NOBRE	UNITED STATES	
39	Lee	PACKER	UNITED KINGDOM	
40	Paul	ROMANO	UNITED STATES	
41	Danila	ROUBTSOV	CANADA	
42	Evgeny	ROZHIKHIN	RUSSIA	
43	Georg	SCHNABEL	AUSTRIA	
44	Stanislav	SIMAKOV	GERMANY	
45	Kristina	SPENCER	UNITED STATES	
46	Kenichi	TADA	JAPAN	
47	Nicholas	THOMPSON	UNITED STATES	
48	Andrej	TRKOV	SLOVENIA	
49	Steven	VAN DER MARCK	NETHERLANDS	
50	Tim	WARE	UNITED KINGDOM	
51	Morgan	WHITE	UNITED STATES	Co-chair

APPENDIX 2

Working Party on International Nuclear Data Evaluation Co-operation (WPEC)
Meeting of Subgroup 45 Validation of Nuclear Data Libraries (VaNDaL) Project

WebEx Meeting

11 May 2020

AGENDA

Duration	PDT (CA, USA)	CEST (Paris)	JST (Tokyo)	Topic	
00:10	05:00	**14:00**	21:00	Welcome	W. Haeck
00:20	05:10	**14:10**	21:10	Review of progress	W. Haeck
00:20	05:30	**14:30**	21:30	Input file QA document	N. Leclaire
00:20	05:50	**14:50**	21:50	Policy driven input file generation applied to MCNP	W. Haeck
00:20	06:10	**15:10**	22:10	Short break	
00:20	06:30	**15:30**	22:30	Development of software to automate the computational analyses of fusion relevant benchmarks	S. Simakov
00:15	06:50	**15:50**	22:50	NRG contribution to the SG45 repository	S. van der Marck
00:15	07:05	**16:05**	23:05	Analysis of ICSBEP U233-SOL Benchmarks	A. Trkov
00:20	07:20	**16:20**	23:20	Delivering a first set of input files	W. Haeck
00:20	07:40	**16:40**	23:40	Discussion	
	08:00	**17:00**	00:00	Close	