IJS Internal Report
IJS-DP-10216
Date: April 2009

THE QUALITY ASSESSMENT OF THE FNG AND TUD BENCHMARK EXPERIMENTS

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I) INTRODUCTION

The scientific community is devoting a constant effort to improve the quality of the nuclear data evaluations for materials that are of interest in the design optimisation of fusion reactors, like the forthcoming ITER. The OECD/NEA Data Bank and ORNL/RSICC joined their expertise in 1996 to produce and maintain SINBAD, the Shielding Integral Benchmark Archive Database. The 'fusion neutronics' section of the project includes the experimental data (radiation shielding and dosimetry) and the computational models relative to integral benchmark experiments relevant for fusion applications. The reviewers and compilers welcome the contributions that reduce the approximations in currently available computational models [1].

The validation of nuclear data libraries relies on computational models that use those for the simulation of integral experiments. The errors in the cross sections evaluations would propagate throughout the bulk material up to noticeable discrepancies with the measurements. The 'fine tuning' of the nuclear reaction channels and their ratios requires the precise assessment of the effect of the nuclear data in the experiment or in different experiments on the same material. The computational models can include, and thus separate, the second and higher affects that are present in the measurements. The MCNP5 code* [2] is the primary computational tool in SINBAD compilation because it allows the realistic modelling of the experimental set–up.

The availability of complete experimental information is a major request for the experiment to be of benchmark quality. The aim of this report is to assess the experimental information available in SINBAD on the contributions from the FNG/TUD collaborations and release a shorthand note on the quality of each FNG/TUD benchmark experiment.

The next paragraph deals with the experimental specifications of the sample assembly, the detector system, the source characteristics and the room structures. There is a fine reduction into the minor items that can be included into the computational models. The lacking or inconsistent specifications are pointed out and, eventually, new references are suggested. The sub–paragraph on the detector system deals with its components and the experimental method. The neutron source specifications are the main object of the present work. They rely on the source subroutines developed at FNG to compile with the MCNP5 source code. The major contribution to the quality of the FNG/TUD experiments is represented by the refinement of the original D–T source model and the validation against bare source measurements. The description of the room structures is considered valuable information for the calculation of the room return effects.

The input files for the MCNP family of codes definitively represent the source of the detailed information on the FNG/TUD experiments. These computational models were developed at the experimental facilities and then are considered a reliable source of information. The improvement of the computational models, which was demanding for the OKTAVIAN and FNS experiments, is in this case not feasible and neither necessary. The structure of this report reflects this issue and the results of the analyses are not reported. A rich literature is contained in SINBAD about the calculations performed by the FNG or TUD team.

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* [1] In general, the same results are also obtained with the MCNPX (version 2.6.f) or the MCNP4 (versions A,B,C). The common choice for the neutron and photon transport problems is the MCNP5 code. For this reason, the MCNP5 is usually recalled even if the input files can be produced for any other code inside the MCNP family of codes (MCNP4A-B-C for the old models or MCNPX 2.6f for the new models).

In the Conclusions, a global quality assessment is elaborated for any benchmark experiment. The experiments of benchmark quality can be used for the validation of modern nuclear data evaluations of the sample material. The experimental specifications of intermediate quality mean that additional experimental information is needed. The approximations are clearly detected and supplementary information is addressed. In this case, the accuracy of nuclear data is not the primary source of uncertainty because of lacking experimental information. The results of the simulations can still be used, but with caution. When it is not possible to develop a model that is useful for the analyses on nuclear data, the experiment is not of benchmark quality.

The references available in SINBAD are quoted with their number in the SINBAD folder and the extensive description of them is given in the References at the end of the report.

The details of the analyses performed on the FNG source subroutines are provided in a separate file. It is an IJS internal report that is included in the SINBAD compilation.

II) EXPERIMENTAL SPECIFICATIONS

The report is directed to readers who possess the SINBAD compilation or have already dealt with the FNG/TUD experiments contained in SINBAD. The description below is not exhaustive because it focuses on the issues that relate to the quality assessment of the experiments. It starts from the information available in the SINBAD folders and directs to the references for more details.

The integral measurements (activation rates and TLD) have been performed at FNG by the FNG team. The neutron and gamma spectra measurements have been performed at FNG by the TUD team. The TOF experiment on the iron slab has been performed at TUD. It is also considered in this report.

The geometry specifications of an experimental component are considered of high quality when all dimensions are specified with a measure (besides the usual tolerance in the design) and the material specifications provide the composition and the density. When some common sense is needed to overcome incomplete experimental information, then the latter is considered of intermediate quality. These roles are forced for the FNG/TUD experiments, but in this way a consistent approach is established with the quality assessment of the OKTAVIAN and FNS experiments in SINBAD.

The experimental specifications are almost completely included in the input files for the MCNP–codes) available in SINBAD. The experimental information on the material samples is detailed, complete and consistent between the spectra and the activation/heating models. The input files have been refined during the years of the experimental activity (1989-2001), mainly to precisely model the monitors. The most recent models include the experimental details to a great extent. They represent a guideline for the analyses of the previous experiments. The original MCNP-4A input files provided in SINBAD for the Stainless Steel and ITER Bulk Shield integral experiments include the geometry and surface cards only. The complete versions of these input files are delivered for the current SINBAD compilation. The major contribution of this work is the study of the FNG neutron source subroutines. It is upgraded and the results are illustrated in subsection II.c. Some experimental features are not included in the computational models depending on the analysis performed or after careful assessment of their negligible effect for that analysis. This issue is underlined in the subsection II.d) because it mainly concerns the room return effects.

II.a) MATERIAL SAMPLE

Besides the many folders in SINBAD database, due to analyses splitting, only six material sample configurations are detected: the W, SiC, ITER Bulk Shield, Stainless Steel Bulk Shield, Dose rate and the Iron Slab assembly. The material sample assembly of the ITER Neutron Streaming experiment is the same as in the ITER Bulk Shield experiments except for the central hole and cavity. The Dose rate assembly, even if close to the ITER Bulk Shield mock–up, differs in the details of the geometry.

The material composition and geometry of the assemblies are completely specified in the computational models. Relying only on the input files is potentially a risk because an independent check of the sample specifications cannot be achieved. An example of high quality experimental information is represented by material specification of the FNG ITER Streaming experiment. For this experiment, the Reference 8 provides the tests performed at ENEA on the chemical composition of the bulk materials. Such a thorough review of the experimental specifications is not usually available for the other experiments. Anyway, since the information contained in the input files is provided by the FNG staff, it can be considered reliable to a reasonable extent. A catch is here recalled concerning the SiC bulk material. The Boron concentration is uncertain and this would affect some calculations, such as the $^{197}Au(n,g)^{198}Au$ reaction rates.

The aluminium support is explicitly modelled in the MCNP-4A input file of the Stainless Steel Bulk shield experiment. The Aluminium movable tower is not explicitly modelled for subsequent experiments. The support model approximation consists of a simplified geometry and an equivalent Al density.

The support structure of the TUD Iron Slab is approximately modelled in the associated MCNP-4A input file.

II.b) DETECTOR SYSTEM

The neutron fluxes in the range E>1 MeV and gamma–ray fluxes in the range E>0.2 MeV were simultaneously measured using a Ne–213 liquid scintillator spectrometer. The experimental information is complete about the detector volume, composition and positioning. Some details on the experimental channel with the preamplifier, photomultiplier, cables are available (see, for instance, Figure 2 in reference 4 of SINBAD folder ‘TUD ITER Bulk Shield’ [3]). The approximate model of the experimental channel is available in the W and SiC MCNP-4C/A input files. The model consists of a C–H homogenous mixture in the realistic volume of the instrumentation channel. The DIFBAS code was employed for unfolding the measured pulse–height distributions in order to generate the neutron spectra and gamma spectra. These were obtained as absolute fluxes. The response function is not required to compare calculations with measurements. For the ITER Bulk Shield experiment, the point–wise flux uncertainty is provided. The systematic and statistical uncertainties are separated. For the W and SiC experiments the total uncertainties of the neutron/gamma flux measurements are provided in energy intervals. The point–wise uncertainties are larger and the average results cannot be used to plot the uncertainty band. This can be considered a drawback in the experimental information.

A second spectrometer system with stilbene scintillation detector and gas-filled proportional counters was employed to measure neutron fluxes in the range 20 KeV<E<1 MeV and gamma ray fluxes in the range 30 KeV <E<0.2 MeV inside the ITER Bulk Shield. The specifications of the parameters of the detectors are summarised in Table 5 of SINBAD folder ‘TUD ITER Bulk Shield’. The uncertainties associated to the detector system are also provided. It is worthwhile to notice that the spectra measurements were in each case corrected for material and size of the detector to a spherical detection volume of 2.0 cm radius filled with SS316 by MCNP calculations with FENDL-1 data. This observation holds also for the Ne–213 detector in the same experiment. Thus, the detector model for the neutron/gamma flux calculations in the ITER Bulk Shield is not approximate but consistent with the measurements.

The detector system in the TUD Iron slab experiment is the same as above for the neutron and gamma spectra measurements in the low and high energy range. The NE–213 scintillation detector was employed for simultaneously measuring the pulse height and the neutron time-of-arrival (or TOF) spectra after the start of the 14 MeV neutron source irradiating the slab. The neutron TOF spectrum and the Ne–213 efficiency curve are provided in SINBAD in computer readable format. The influence of room-return and other background components is assessed. The information on the multiple scattering effects is correctly contained in the TOF spectra. Thus, the conditions for the TOF experiment to be of benchmark quality (see for instance the report on the OKTAVIAN experiments) are met. The neutron spectra in the energy domain are obtained by unfolding the pulse height spectra, so they are not affected by any conversion method from time into energy domain. The statistical and systematic uncertainties are separated and provided for the efficiency function and for the spectra in the time domain and in the energy domain.

The activation foils are inserted into the sample assemblies in specified positions. The foil materials can be inferred with some common sense, thus neglecting impurities. The Al holder and air layer around the foils are explicitly included in the MCNP-4C input files for the W activation analyses. The specification of the foils sequence arrangement, if any, is not available for the SiC case. The radiometric technique is described providing the sources of uncertainty that contribute to the total uncertainty of the activation rates measurements.

The result of the analyses would indicate that some activation measurements might not be considered reliable (for instance, the Mn activation in the W experiment, Au in Sic experiment and in ITER Bulk Shield).

For the ITER Bulk Shield experiment, the coherence between neutron flux and activation measurements was established (reference 13 in the SINBAD folder ‘TUD ITER Bulk Shield’ [4]). The same coherence test is also available for the ITER Streaming experiment [4]. The spectra measurements of the TUD-ITER Neutron Streaming experiment are not compiled in SINBAD. The references on the spectra measurements are available in the SINBAD folder ‘FNG-ITER Neutron Streaming (integral)’, for instance reference 6 in this folder. The coherence test in the Neutron Streaming experiment is not clearly passed [4]. The re-calculation of the activation rates with the MCNP-4A model available in SINBAD folder are in disagreement with the results available. P. Batistoni, the author of the original analyses, provided the new MCNP5(X) input file to reproduce original results. Concerns about the coherence between the spectra and activation measurements in the W experiment are advanced by dr. Trkov [5].

The material composition, geometry and positioning of the TLDs are specified. The experimental method is provided.

II.c) SOURCE

The geometry and material composition of the FNG target assembly are completely specified in the MCNP–codes input files. The target assembly consist of the Ti–T pallet, the copper cup, the water cooling system, the ion tube. The ion tube model is 255 cm long for the

Stainless Steel Shield and ITER Bulk Shield (flux analysis) and 14 cm long in all the other cases. The ion tube approximation was duly introduced after assessment of the negligible effect of the most distant part of the tube.

The SINBAD database makes available the subroutines to compile with MCNP4C (original version), MCNP5 and MCNPX source codes for the simulation of the neutron emission in the Frascati Neutron Generator. The source model provides the neutron source energy distributions and yields at any direction. The tables from the MCNP-4B version are available in SINBAD with the equivalent source neutron spectra and yields at 10° intervals. The SINBAD compilations of the oldest experiments (Stainless Steel Shield and ITER Shield/integral measurements) contain the table with the source neutron spectrum averaged over a spherical cap of 60 degree aperture. This approximation is not anymore necessary. The measured source spectrum is not given in the FNG/TUD folders. The detailed information on the source subroutines validation is not directly available in SINBAD. The author M. Pillon suggested his paper [6] for the purpose.

The features of the FNG source model are generally described, for instance, in SINBAD ITER Bulk Shield/integral reference 2 [7]. The source model includes the realistic effect of the deuteron slowing down inside the Titanium–Tritium target and the D–T reaction kinematics. It is based on the 'Stopping and Range of Ions in Matter' code (SRIM2006 [8], http://www.srim.org/). SRIM is a well established collection of software packages (TRIM is the for ion transport) that calculate many features of the transport of ions in matter, such as ion stopping and range in targets, ion implantation, sputtering, ion transmission, ion beam therapy. SRIM was developed since the 90's by J. F. Ziegler, J. P. Biersack and M. D. Ziegler. M. Pillon translated into Fortran language part of the statements of the old version (1996) of TRIM, which was written in basic language. These statements model the deuteron ion transport inside the target. There is a strict parallelism between the source routine and the TRIM version. TRIM does not model nuclear reactions. M. Pillon implemented the original part concerning the neutron production. The D–T reaction data are those from the DROSG2000 code ([9], http://www-nds.iaea.org/drosg2000.html). The essential characteristics of the FNG source model (MCNP-4C version) are sketched in the following list:

1. Monte Carlo method for D transport,
2. free flight paths between D collisions, which 'condense' negligible amounts of energy transfer and deflection angles,
3. impulse approximation for the free flight paths in the D low energy range,
4. universal interatomic potential,
5. Rutherford scattering at higher ion energies,
6. electron stopping power data from the TRIM code tables,
7. D–T integral cross sections retrieved from the DROSG2000 code calculations at different deuteron energies
8. neutron generation by the modified Von Neumann rejection method,
9. classical kinematics.

The source subroutines are SOURCE.F90 (coding the D slowing down in solid Ti–T target and modelling the fusion reactions), SRCDX.F90 (specific for transporting neutrons generated in SOURCE to point detectors) and six other subroutines for numeric calculus. The source model requires the use of the RDUM card in the MCNP input file to specify: deuteron beam energy, target thickness, T/Ti atomic fraction, beam width, target axis coordinates.

The last version of the source model was prepared at FNG for the MCNP5 code. A patch file is produced that is included in the new SINBAD compilation. The patch file is to apply to the original MCNP5 source code for WINDOWS and LINUX systems. The text format (UNIX or PC) of the source and patch files have to be consistent. It is now possible to perform routine calculations on WINDOWS and LINUX systems in the sequential mode. The parallel mode has also been tested in the MPI and OMP environments. These compilations perform well but the test with the point detector in parallel mode cannot be passed. It is noticed that the parallel mode is usually needed for complex calculations that make use of cell flux detectors.

An unphysical spike at the deuteron maximum energy appeared when calculating the neutron spectra on a very fine energy binning with the FNG source model [10]. After discussion with M. Pillon the special treatment of the first collision (item 2 of the list above) is dropped and the spike disappears [11] [2].

The range of the deuterons in the last version of the source model was underestimated with reference to the TRIM calculations. The problem has been found in the stopping power of the Ti–T mixture (item 6 of the list above). Since the units of the data imported into the routines from TRIM tables changed from the original MCNP4B version, some parameters needed to be modified accordingly. It is now possible to ascertain that the mean average range of the deuteron ions is about 1.5 μm in the new version, about the same value given by the TRIM code [11].

An original condition is implemented into the SOURCE subroutine to terminate the Monte Carlo history when the cumulative deuteron free flight path exceeds the target thickness [11].

The integral D–T cross sections in MCNP4B version (item 7 of the list above) were upgraded to double differential in the MCNP5 version by FNG. The data were still retrieved from DROSG2000 calculations. The use of double differential cross sections in the source model had two drawbacks. First, it was not easy to check if any data were wrong or approximate because the data section was huge. Second, the cross section data relied on DROSG2000 Legendre coefficients, which could change according to new experimental evidence or refinement of theoretical nuclear models. The source subroutines are modified to generate internally the double-differential cross sections from the integral cross sections and the Legendre coefficients available in the ENDF/B-VII nuclear data library (MAT=2, MF=50, MT=3,6 [12]). The new version has been validated with the past MCNP5 version [11].

The source subroutines are further improved to introduce the relativistic kinematics of the ^{3}H(d,n)^{4}He reaction (item 9 of the list above). The use of relativistic kinematics results in a shift of about 30 KeV to lower neutron energies [11].

The modifications introduced in the new MCNP5 version required a revision of the SRCDX subroutine for point detectors. A cross-validation of the source model is performed comparing the cell flux estimator and the point detector source neutron spectra. It is found that both tallies are consistent [11].

The FNG experiment on the type IIa diamond detector [6] is an ideal test case for the upgraded source model validation because the source is bare. It was carried out with the bare ~14 MeV neutron source. M. Pillon provided the raw experimental data, which are the counts per channel of the measurements. The transformation into the energy spectra is performed applying the calibration formula and the energy shift of 5.7 MeV, which is due to the kinematics of the ^{12}C(n,α_0)^{9}Be reaction in the diamond detector. The detailed MCNP5 model of the FNG neutron generator and experimental room is used to reproduce the measured spectrum using point detectors at the diamond detector positions at 0°, 95° and 172.5°. The energy of the accelerated D is 230 KeV M. Pillon also provided the output file of the calculation carried out with the MCNP4B version source model (‘MCNP4B VERSION’).

[2] The original results presented in this paragraph and in the references were obtained by dr. Trkov. My personal contribution was the improvement of the source subroutines and the preparation of the input files.

Thus, the spectra obtained with the upgraded MCNP5 source model ('MCNP5 REVISED VERSION') are compared both with the ones retrieved from Pillon's output file and with measurements (Figure II.c–1). The tails in the measurements below the ~14 MeV peak are due to the incomplete charge collection in the diamond detector, which cannot be reproduced with the point detectors in MCNP5. A 1 % FWHM Gaussian broadening is applied to calculated spectra to reproduce the experimental energy resolution. The spectra are normalised to the maxima of the measured spectra and the same scaling factors are applied to the calculations with the MCNP4B and MCNP5 REVISED version of the source model. The energy binning is finer in the latter case, as can be seen for the 172.5° spectra. In the backward direction the MCNP5 source model provides a spectrum somehow shifted towards higher energies. It is worthwhile to notice that the neutron emission in the backward direction is not much important in the FNG experiments. The shapes of the calculated peaks are in fair agreement with the measured ones. The spectrum calculation in the forward direction is preferable after the improvements implemented in the FNG source subroutines. The distance between the 0° and 90° peak maxima is well reproduced in the simulation.

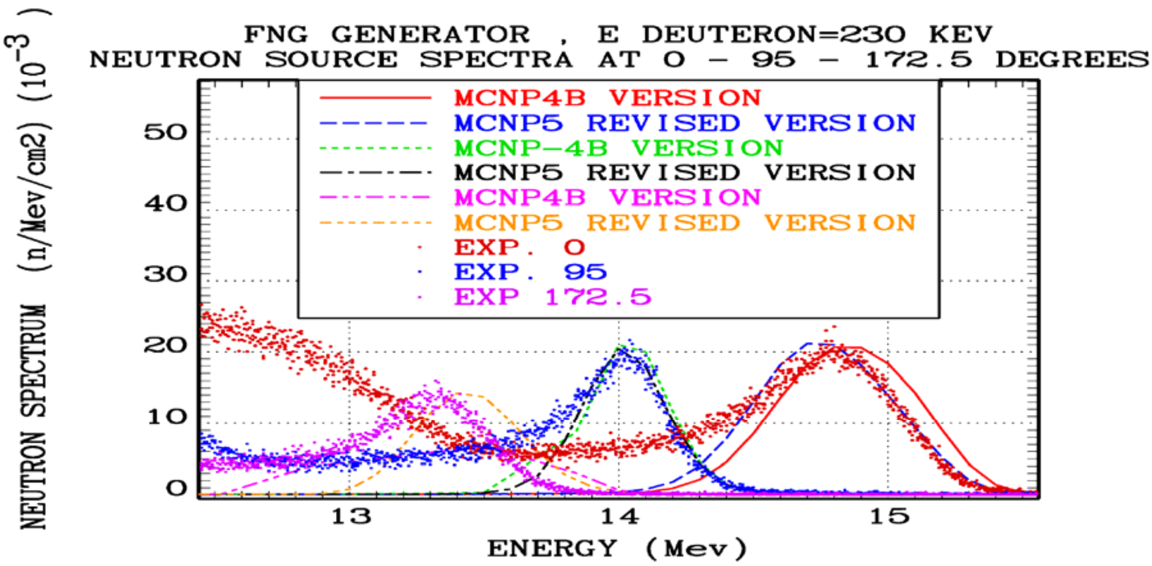

Figure II.c–1. Diamond detector spectra simulations: comparison between results obtained with the original MCNP-4B version and with the new MCNP5 version

The source specifications for the TUD iron slab experiment consist of the equivalent calculated neutron source spectra at 10° intervals and associated yields. The information on the time uncertainties is modelled in the MCNP5 input file by the Gauss time distribution of the source neutrons. It is not possible to simulate the neutron source spectra specifications based on the available information in SINBAD. The TUD source spectra specifications can be considered reliable after observing the agreement, especially at the elastic peak, between measured and calculated TOF spectra.

II.d) ROOM

The room return effects are included in the MCNP–codes models for the spectra calculations. The only sample assembly in included for the integral measurements simulations. The effect of the room return is assessed in the case of the Stainless Steel Bulk experiment.

III) CONCLUSION

A major collection of integral experiments for fusion applications is preserved in the Shielding INtegral Benchmark Archive Database (SINBAD). The Italian facility FNG contributed to the database with the integral measurements (activation rates, heating, dose rates) on ITER-related structures and materials. Some of the experimental sessions foresaw the TUD expertise to perform neutron and gamma spectra measurements. Moreover, a TOF leakage spectrum experiment on Iron slabs, performed at TUD, is also considered here. The information from the original documentation has been organised, compiled and reviewed within the SINBAD. The outcome is a user–friendly presentation of the benchmark information, including the computational models for the simulation of the experiments.

The completeness and consistency of the experimental specifications for the sample geometry and material composition have been verified. A drawback is noticed concerning the availability of almost full experimental information in the original computational models. An independent source of experimental information would be advisable.

The experimental specifications of the neutron source at the FNG are considered of high quality because the simulation of the neutron source measurements is feasible. The simulations are performed with the source subroutines to be compiled with the source codes of the MCNP-family. The source subroutines have been refined and their usage updated to the MCNP5 code. The source specifications for the TUD Iron Slab experiment are also considered reliable (and thus of benchmark quality) because in this case the neutron source term can be indirectly validated, for instance with the sample–in–place measurements at the elastic peak.

The realistic computational model for the FNG/TUD experiments have been developed, including the details on the detector system and, whenever necessary, on the experimental room.

The measured spectra for the W and SiC experiments include information on the uncertainties in energy intervals. The point–wise uncertainties are advisable for modern data validation.

The issues above (sample, source and detector specifications) are considered as the most important to assess the quality of the FNG/TUD experiments for the modern nuclear data evaluations

A note is finally released on the quality assessment on any FNG/TUD experiment available in SINBAD compilation (fusion neutronics section). The note is synthetic to assist the users in properly selecting the benchmarks from the database.

THE IRON SLAB EXPERIMENT IS RANKED AS **BENCHMARK QUALITY EXPERIMENT**

THE STAINLESS STEEL BULK SHIELD EXPERIMENT IS RANKED AS **BENCHMARK QUALITY EXPERIMENT**

THE ITER BLANKET BULK SHIELD EXPERIMENT IS RANKED AS **BENCHMARK QUALITY EXPERIMENT**

THE ITER NEUTRON STREAMING EXPERIMENT IS RANKED AS **BENCHMARK QUALITY EXPERIMENT**

THE ITER DOSE RATE EXPERIMENT IS RANKED AS **BENCHMARK QUALITY EXPERIMENT**

THE SILICON CARBIDE EXPERIMENT IS RANKED AS **BENCHMARK QUALITY EXPERIMENT**
Supplementary experimental information is advisable on:
– The neutron and gamma flux point–wise uncertainties

THE TUNGSTEN EXPERIMENT IS RANKED AS **BENCHMARK QUALITY EXPERIMENT**
Supplementary experimental information is advisable on:
– The neutron and gamma flux point–wise uncertainties

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