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FENDL Library for Fusion Neutronics Calculations

Summary Report from the Consultants' Meeting
IAEA Headquarters
15-18 October 2018

Lee Packer
UK Atomic Energy Authority
D3 Culham Science Centre

Andrej Trkov
IAEA
Vienna, Austria

December 2018

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

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Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

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Contents

The participants were welcomed by Arjan Koning, Head NDS, who outlined the IAEA's involvement in fusion and emphasised the reliance of the fusion community on the FENDL library.

Ulrich Fischer was proposed chairman and Lee Packer Rapporteur by the Scientific Secretary of the meeting, Andrej Trkov. No objections were raised from the participants.

1. Introduction

Andrej Trkov stated the objectives of the meeting, which are to assess the performance of the current FENDL 3.1d library, and to also assess the FENDL-A (activation) library and the next release of a library, whether that be FENDL3.1e or a more significant FENDL4.0 release. He outlined some of the historical problems identified with FENDL libraries which has impacted e.g. on the heating in concrete (K-39 in 3.1c, improved in 3.1d) and what other aspects of the library might be wrong. He emphasized that 'newer is not always better' for a specific evaluation. A discussion followed whether a FENDL4.0 library should be introduced, or just minor improvements be made.

2. Summary of presentations by participants

2.1 Processing nuclear data for FENDL-2.1 and FENDL-3.1d, D. Lopez Aldama

The history of FENDL from version 2.1 up to 3.1d was presented. The main issues concerning evaluation problems and processing options were analyzed. The differences between the processing options of FENDL-2.1 and FENDL-3.1d were discussed with emphasis on Doppler Broadening, probability tables and kinematic KERMA calculations. The quality assurance procedure for trapping processing errors was also explained. It was concluded that FENDL-3.1d is available and its limitations are well known. It was suggested to evaluate the possibility to update the library to version 3.1e or 4.0 to improve the analysis of fusion systems for ITER and DEMO, and to material test facilities such as IFMIF.

Various problems were identified by C. Konno at the previous meeting, which are discussed below.

<u>Problem 1:</u> O-16 data should be replaced above 20 MeV by JENDL/HE-2007 or other evaluated nuclear data. Recommendation is to replace O-16 data >20MeV with JENDL4.0/HE. (Action: SK)

<u>Problem 2:</u> Missing angular energy distribution over 20 MeV for several MATXS files like Fe-56. This issue was due to a processing error in NJOY and has already been corrected in version 3.1b.

<u>Problem 3:</u> Problems with KERMA
Problems due to an issue in NJOY have been corrected.

<u>Problem 4:</u> Non-monotonically decreasing energy boundaries in MATXS formatted files for some isotopes. This was due to an issue in NJOY and has been corrected.

<u>Discussions following the presentation</u>:

Trkov commented that covariance data are rather limited. A future version of FENDL with full covariance data will be required for uncertainty assessments.

Trkov showed the IAEA FENDL webpage and how to access various files, per isotope.

The origin of K-39 problems in FENDL3.1b was outlined. The problems were corrected in FENDL-3.1c and FENDL-3.1d, the latter being the current recommended version.

An incompatibility between MCNP5 and the FENDL-3.1d ace library for some isotopes was found by the ITER Organisation which caused an infinite loop in MCNP5. It was noted that no such compatibility issues exist with MCNP6. A list of these problematic isotopes exists at F4E. (Action MF: to detail a description of the specific problem in MCNP and to distribute the list of isotopes with this issue to the participants). The list was already provided before the end of the meeting and contained many materials, including Fe-56. However, test calculations including only Fe-56 could not show the problem, so the error needs further investigation to identify the offending material.

2.2. The Impact of ENDF/B-VIII.0 and FENDL-3.1d data on fusion neutronics calculations for ITER, T. Bohm

The main points discussed in the presentation were:

- Radiation levels in three models of D-T fusion devices were determined using 3 separate neutron transport libraries with the MCNP radiation transport code. The impact of photon libraries was determined in previous work.
- The three models were a 1-D model of ITER, a 3-D model of ITER, and a 3-D model of the U.S. Fusion Nuclear Science Facility.
- ACE neutron libraries from FENDL-2.1, FENDL-3.1b/d, and ENDF/B-VIII.0 were used.
- Neutron flux, photon flux, dpa, gas production (He, T), neutron heating, photon heating, and total nuclear heating levels were determined in various components in the models.
- The maximum differences observed between the libraries used as compared to FENDL-2.1 are the following:
    - Neutron flux 12%
    - Photon flux 22%
    - Dpa 9%
    - He production 18%
    - Total (neutron+photon) nuclear heating 14%
    - Neutron heating 70%
    - Photon heating 9%
    - Tritium production in structural material 200%
    - Tritium breeding in PbLi breeding material 1.7%
    - Note: not all radiation quantities were determined for all models at all component locations.
- Future work can include calculation of radiation levels at more locations in the individual models and calculations of more radiation quantities in the individual models.

FENDL3.1d provides a conservative estimate in several cases, but the origin of the cases should be studied. Different behaviour has been observed in using the ENDF/B-VIII.0 library. Some key isotopes in the ENDF/B-VIII.0 have been updated. Trkov commented that Fe-56 and the Cu isotopes were not necessarily better than FENDL-3.1 for fusion neutronic calculations. An updated ENDF/B-VIII.0 Fe-56 file is in preparation at the IAEA.

In the discussion relating to photon data libraries in FENDL/MCNP, historically less effort has been spent on the photon data. This is particularly important for photon heating. Previous work has shown that the standard MCNP library, mcplib84 or later versions, correct a bug in mcplib04. mcnplib84 is therefore the recommended photon library.

A new photon library is available in mcnp6.1, epr12 and for MCNP6.2, epr14. these libraries include low energy < 1 keV data. It is suggested that these libraries are not particularly relevant to typical fusion neutronics assessments.

The objective is to look at the impact of using the updated neutron libraries in a realistic model of fusion systems. For this purpose the ITER 1-D cylindrical benchmark developed by M Sawan in 1994 (reported in INDC(NDS)-316) can be used.

Compared nuclear quantities (e.g. flux) as a function of radial cell number for all four libs with FENDL2.1+84p i.e. 31b+84p, 31d+84p, 80c+84p, 00c+84p were presented.

Conclusions and future work:
Future work – examine cross sections directly, use detailed ITER 3D model with less homogenisation, examine more radiation quantities and location in FNSF and ITER 3D models.

Discussions following the presentation:
It was proposed to conduct a substitution study to identify, isotope by isotope, what is the cause of the differences between FENDL-3.1d and ENDF/B-VIII.0 are. The material which is responsible for the observed large difference with ENDF/B-VIII.0 needs to be identified. Some suspicion is that the problem lies with ENDF/B-VIII.0 and not FENDL. (Action: TB)

2.3. New comments on data below 20 MeV in FENDL-3.1d, Ch. Konno

Konno presented a range of new problems on FENDL-3.1d identified since the last FENDL meeting in 2016. His presentation was divided into five sections, discussing each of the problems. These are summarised below:

(1) Problems on KERMA and damage energy of ^{39}K and ^{40}K in FENDL-3.1d

Reasons of difference between kinematics and energy-balance KERMA factors of ^{39}K in FENDL-3.1b (TENDL-2012) and -3.1d (TENDL-2015) were discussed in detail. The following issues were found:

- This issue is not due to NJOY, but due to the ^{39}K data themselves of FENDL-3.1b and -3.1d.
- Secondary gamma yield and energy distribution data of secondary alpha, residual nucleus and secondary gamma of the (n,α) reaction in ^{39}K of FENDL-3.1b and -3.1d seem to be incorrect. This causes this issue and leads to the wrong damage energy.

The ^{40}K file in FENDL-3.1b (TENDL-2012) and -3.1d (TENDL-2015) also have the same problem. It was noted that the same issue also occurs in ^{39}K and ^{40}K in TENDL-2017. Additionally, it was pointed out that the ^{40}K and ^{41}K data in FENDL-3.1d are not identical to those in the TENDL-2015 official site.

Discussions relating to these issues:
The first issue relating to K-39 in FENDL-3.1b was due to incorrect resonance parameters and was fixed in FENDL-3.1c. However, the problem with secondary alpha and gamma at energies below 2 MeV in K-39 remains.

It was concluded that the evaluated data files need to be corrected. The solution to this problem involves replacing the secondary alpha and residual nucleus of the (n,α) reaction dd data at 1e-5 eV with data at 20 keV and the secondary gamma of the (n,α) reaction < =2.2 MeV with data at 2.6 MeV and modifying the secondary gamma yield < 2.6 MeV such that the energy balance is preserved. (Action: C. Konno will provide a corrected file)

Other nuclides taken from TENDL containing threshold reactions with positive Q-values should also be checked. (Action: C. Konno)

(2) Problem on p-table in ACE file of FENDL-3.1d

It was examined why heating number probability tables (p-tables) of 33 nuclei in FENDL-3.1d ACE were negative. The reason of the negative p-table was because the problematic nuclei have no secondary gamma data of the capture reaction or secondary gamma data of the capture reaction in the nuclei are stored in file12-15 mt=3, not mt=102. The self-shielding effect for KERMA in the unresolved resonance region are very small. In order to eliminate negative p-tables, C. Konno proposed a method to set the heating number p-table to "1.0" or an average heating number without calculating the partial KERMAs of the elastic scattering, fission and capture reactions in the HEATR module.

Discussions relating to this issue:
It was concluded that the ACE files need to be corrected. A patch for the ACER module (for the second run) should be created to fix this issue. It was decided that MATXS files are to be left as they are. (Action: D. Lopez Aldama)

(3) Problem on MATXS file of FENDL-3.1d due to NJOY unresolved resonance processing

C. Konno encountered a problem in a simple calculation for a Lanthanum sphere with ANISN and the MATXS file of FENDL-3.1d. It was found out that unrealistic, too small, cross sections between resonances in ladders for unresolved resonances caused large self-shielding corrections, which is the origin of this problem. As a trial, NJOY2016 was modified to eliminate unrealistic cross section features in the dips between resonances. In this approach MATXS files with the modified NJOY2016 gave better results. In addition, the ACE files that were produced with the modified NJOY did not affect MCNP calculation results.

Discussions relating to this issue:
These issues were noted though an action was not deemed to be essential because in practical situations it is unlikely to find Lanthanum in large quantities that would result in such strong self-shielding.

(4) IAEA patch effects for TRANSX

Effects of the first of the IAEA unofficial patches for the TRANSX2.15 code were examined with a simple calculation model and the MATXS file of FENDL-3.1d. Findings are as follows:

- Large neutron fluxes appear in calculation results with self-shielding corrected multigroup libraries produced by the original TRANSX2.15 code. This effect is larger for lighter nuclei.
- The first IAEA patch solves this problem, it should be modified for MATXS files with a larger number of neutron groups.

Additionally, two issues were reported.

- A bug of TRANSX2.15 for FENDL-3.1d ^{56}Fe.
- Inadequate background cross section data in the FENDL-3.1d MATXS file.

Discussions relating to this issue:
The IAEA patch that was produced for TRANSX2.15 is adequate for the FENDL-3.1 MATXS library in 175 and 211 neutron energy groups. However, the patch is not suitable for finer group structures such as the 640 neutron energy group structure.

An additional patch for TRANSX2.15 is needed to process Fe-56. (see simple modification in C Konno presentation slide 66)

It was recommended that the IAEA TRANSX2.15 patches should be included in the current FENDL website. (Action: AT)

A lower background cross section value should be added to generate MATXS files, for example in Na-23, Mg-24, Mg-25, Mg-26, Al-27, Si-28, Si-29 and Si-30. However, other nuclides should be checked as well. (Action: D. Lopez Aldama)

(5) Comments on TENDL-2017

It was pointed out that secondary gamma spectra from the capture reaction from a lot of nuclei in TENDL-2017 had fewer high-energy gamma peaks than those in other nuclear data libraries. This problem causes smaller gamma fluxes in neutron-gamma coupled calculations than those with other nuclear data libraries and much smaller DPA cross-section data. Two additional issues were reported, which were:

1) Two ACE file sets from the TENDL-2017 website are different: one is a .tar file of all ACE files and the other contains individual files. There is no information showing the differences on the website. The individual files do not include probability tables (produced using PURR) and secondary gammas.
2) There is no gamma production data in the TENDL-2015 ACE files on the TENDL website, but this issue is not thought to be relevant to FENDL as the files were processed separately.

Discussions relating to these issues:
Koning commented that PGAA gamma lines are not in the TENDL library (but are in e.g. ENDF/B libraries). A way to automatically include this in the assembly of future TENDL libraries needs to be found. This is relevant to the TENDL nuclides already adopted by FENDL in the current version.

2.4. Significant comments on data above 20 MeV in FENDL-3.1d, S. Kwon

The new intense fusion neutron source, A-FNS, is an ongoing project for irradiation tests of fusion DEMO reactor materials in Japan. QST is the organization in charge of the design activity and the irradiation test plan development of A-FNS. A-FNS produces a large number of neutrons via the d-Li stripping reaction and the maximum neutron energy is expected around 55 MeV. QST have used FENDL-3.1 for neutronics calculations of A-FNS.

QST investigated FENDL-3.1d in detail through DPA cross section data and analyses of QST/TIARA iron shielding experiments. In the presentation the problems of the DPA cross section and the secondary neutron spectrum data above 20 MeV were described.

DPA cross section data issue

In the DPA cross section data above 20 MeV, it was found that a lot of DPA cross sections above 20 MeV in FENDL-3.1d had problems. It was identified that production yield data of several residual nuclei in ^{56}Fe were not correct at 20.00001MeV and the incorrect data made a sharp spike just above 20 MeV in the DPA cross section of ^{56}Fe, caused a questionable DPA ‘dip’. In addition, an examination of all the DPA cross section data above 20 MeV in FENDL-3.1d was performed. The results are summarized in the Table below. The DPA cross section data of more than 70% of nuclei in FENDL-3.1d have problems because of defects of the original nuclear data.

Energy region	Problem of DPA cross section	Number of Nuclei		Source data
Above 20 MeV	Sharp negative spike	4	74	OLD TENDL data (TENDL-2010, 2011)
	Large peak	7		
	Sharp spike	63		
	Sharply small	49		JENDL/HE-2007
Above several MeV	Much smaller	13		JEFF-3.1.1

Discussion relating to the three dpa issues:

- Issue 1: The narrow dip in dpa at 20 MeV exists in 74 nuclei (FENDL-3.1d which are taken from the TENDL-2010/11 files). Modifications to the residual production data are needed in MF6. (Action: A. Trkov)
- Issue 2: The DPA cross section shows a discontinuity (a sharp drop) around 20 MeV. This is seen e.g. in Nb-93 (FENDL-3.1d which is taken from the JENDL HE file). A similar issue exists in 49 nuclei. The issue is that energy distribution data of residual nuclei above 20 MeV are missing. This was identified as a significant problem that is not straightforward to resolve. In the interim period it was suggested to use alternative dpa data libraries e.g. JEFF-3.3, if needed above 20 MeV.
- Issue 3: The DPA cross section shows a decline starting around 2-3 MeV. This relates to the DPA cross sections of 13 nuclei from JEFF-3.1.1 in FENDL-3.1d. It is suggested to replace these nuclides with JEFF-3.3.

Secondary neutron spectrum issue

In the secondary neutron spectrum data at 20 MeV it was discovered that the calculated neutron fluxes using FENDL-3.1d unnaturally increase near 20 MeV. The reason for the increase was due to incorrect secondary neutron spectrum data at 20 MeV in the ^{56}Fe data contained in FENDL-3.1d, which were taken from an old TENDL library, TENDL-2011. TENDL-2017 had a similar problem, which occurs near 30 MeV and is caused by the incorrect secondary neutron spectrum data at 30 MeV of ^{54}Fe, ^{56}Fe and ^{58}Fe in TENDL-2017. A lot of additional data in TENDL-2017 and TENDL-2015 have the same problem. Kwon stated that she hopes that FENDL-3.1d will be revised as soon as possible based on this study.

Discussions on the secondary neutron spectrum issue:

After checking the original TENDL-2010 files it was found that the neutron spectra at the breakpoint energy, when the transition to lumped reaction MT5 is made (and at a small increment in energy), are systematically wrong in all versions of the TENDL libraries that were spot-checked. Backward extrapolation from higher energies is dangerous due to the difficulty of properly defining the maximum energy and the average energy of the spectrum. The use of another version of the TENDL library is not applicable, since they mainly have the breakpoint at higher energies; there is no library with a breakpoint below 20 MeV that could be applicable. An alternative exists for iron in the INDEN evaluation from the IAEA, but no such solution is available for the other nuclides.

2.5. Recent Evaluation/benchmark works in the JENDL project relevant to FENDL, S. Kunieda

S. Kunieda (JAEA) gave a presentation about recent evaluation and benchmark works in the JENDL project. Firstly, he talked about new libraries which have been released since FENDL-3.0 was completed. One of the new libraries is JENDL-4.0/HE library in which the nuclear model code CCONE was applied to estimate cross-sections up to 200 MeV for incident neutrons and protons (JENDL-4.0 was adopted for incident neutron data below 20 MeV). With advanced nuclear models such as Iwamoto-Harada model, the evaluated data shows reasonable agreement with measured data not only for nucleon production but also composite-particle and residual nuclei production cross-sections. The library also includes new evaluations for p+^{6,7}Li and p+^{9}Be where the (p,xn) double differential cross-sections are carefully estimated by the interpolation of available experimental data with suitable nuclear models. He also touched on a new activation cross-section library JENDL/AD-2017 in which neutron cross-sections on 311 isotopes are included up to 20 MeV. Those libraries are already available on the web site of JAEA Nuclear Data Center (also on the web site of IAEA-NDS).

S. Kunieda also presented ongoing studies on the evaluation work conducted at the JAEA. The DEURACS code had been developed to estimate deuteron-induced reaction cross-sections. With this code, which is based on the CCONE code coupled with CDCC+Glauber model, it predicts cross-sections fairly well. It should be noted that the break-up reaction is well simulated by the code, so the calculated (d,xn) spectra are in good agreement with measured data. There is a plan to produce a deuteron induced data file in ENDF-6 format, which could be considered for inclusion in a future FENDL library.

JAEA have also produced a photo-nuclear data library, JENDL/PD-2016. This library can also be considered for future use in FENDL.

Finally, he talked about the present status on the development of JENDL-5. The library is now under development focusing on the updates of neutron cross-sections for light-nuclei, structural materials, fission products and actinides. In this meeting, some improvements from JENDL-4.0 were shown for structural materials such as copper. They also plan to add isomer production cross-sections and covariance data as much as possible. The forthcoming data library will be released, expected in 2021.

2.6. Nuclear data validation efforts – Decay heat validation of the FENDL activation library, L. Packer

Lee Packer outlined the validation effort carried out at UKAEA Culham performed on activation files using the FISPACT-II code, a multiphysics inventory code (see “FISPACT-II: An Advanced Simulation System for Activation, Transmutation and Material Modelling” Nucl. Data Sheets 139 (2017) 77137). The full validation reports are available at: http://fispact.ukaea.uk. A suite of automated validation benchmarks have been created to test new releases of both the FISPACT-II code and the nuclear data libraries, particularly focussing on TENDL-2017 and FENDL-3.0/A as well as other libraries.

The presentation focussed on using the very valuable Japanese FNS experiments that were carried out between 1996 and 2000 (see F. Maekawa M. Wada, Y. Ikeda et al. Tech. Rep. JAERI-Data/Code 98-024, JAERI-Data/Code 98-021, & JAERI 99-055. http://www.jaea.go.jp/jaeri/), where thin samples of a range of materials, 25x25 mm^2 in area, and typically 10 µm thick, were irradiated, either as metallic foil or powder sandwiched between tape. 14 MeV neutrons are generated in the FNS by a 2 mA deuteron beam impinging on a stationary tritium-bearing titanium target. The total neutron flux at the sample location, for this experiment, is in the range of 1E10 [n cm−2 s−1]. The irradiation time at the FNS were either 5 minutes or 7 hours. The decay energy in each irradiated sample was measured in the Whole Energy Absorption Spectrometer (WEAS), which comprises two large bismuth-germanate BGO scintillators in a geometric arrangement, provides almost 100 % detection efficiency for both β and γ-rays. The detection system was housed in low background shielding.

Detailed experimental information (irradiation times, measurement times, material compositions, etc.) have been translated into a set of FISPACT-II input files to perform corresponding decay heat calculations using the FENDL-3.0/A activation library (which is identical to EAF-2010) and a range of other libraries, notably including TENDL-2017, but also ENDF/B-VIII.0, JEFF-3 and IRDFF1.05.

Example results were shown for Fe irradiation and comments on library performance were made.

For the Cu the 5 minutes irradiation experiment there is good agreement, within a few % at all decay times. The dominant reaction product is Cu-62.

For the palladium the 5 minutes experiment the TENDL-2017 library outperforms all the others. This is a complex case with many contributing nuclides, particularly the metastable isotopes Rh-108m, Pd-109m and Rh-106m. The FENDL3.0/A library overpredicts Rh-108m. The ENDF/B-VIII.0 and JEF3.3 libraries miss important isomers and consequently significantly underpredict the experimental result.

For the Iridium the 5 minutes irradiation the FENDL3.0-A library performed the best. It is thought that there may be some misattribution of isomeric states in the TENDL-2017 file.

For the indium experiment all of the libraries show poor agreement with the experiment. The incorrect allocation of the In-115(n,g) to In-116, In-116m and In-116n may be a possible explanation. An alternative possibility is that the thermal part of the FNS experiment is poorly characterised (C. Konno raised the suggestion that concrete might not have been included in the original MCNP modelling of the spectrum which were used as input to the FISPACT-II calculations).

Summary tables of the full decay heat results are presented in the main report (https://fispact.ukaea.uk/wp-content/uploads/2016/06/CCFE-R1525.pdf).

It was pointed out that other aspects of the activation file validation are considered alongside decay heat validation, such as integro-differential validation, Fission decay heat.

Discussion

There was some discussion on the astrophysics validation using KADONIS and Maxwellian averaged cross sections (MACS). A. Trkov raised some objections to the way in which KADONIS was used for this work. It is well established that the MACS for gold in the official KADONIS database is too low. This is a problem because gold was often used as a standard for other relative cross section measurements. There exists KADONIS version 1, but it is labelled as “work in progress”. The normalisation to the Standard was to some extent corrected, but it is not clear if it was applied throughout. Furthermore, in the example of Fe-56 several measurements are reported, but the lowest one is adopted, which happens to coincide with the values from practically all major libraries. However, this apparent agreement is not too surprising since all libraries adopt almost the same resonance data, with only minor corrections in some cases. The recommendation by A. Trkov was to use the KADONIS database with caution and use Version 1 in preference to the official KADONIS database.

Regarding the activation library, the recommendation is to introduce a TENDL-2017-based activation library (or later version, if available and tested) as the substitute for FENDL 3.0/A sub-library in a future release of the FENDL library.

2.7. INDEN (post-CIELO) Fe-56 evaluation, A. Trkov

A. Trkov presented some recent results of the benchmarking of the Fe-56 evaluation containing improvements implemented after the release of the CIELO files, which were adopted in the ENDF/VIII.0 library. Initial testing of the CIELO files was done primarily on the criticality benchmarks. After the Fe-56 file was "frozen", validation work continued. S. Simakov found a serious deficiency in the performance of the Fe-56 file in modelling the leakage spectra from a thick iron shell with a Cf-252 source in the centre. The ENDF/B-VIII.0 library underpredicts the spectrum in the 1-5 MeV range. This deficiency was acknowledged already in the report that described the contents of the ENDF/B-VIII.0 library (See Nuclear Data Sheets, 148 (2018) 214-253).

Improvements to Fe-56 were elaborated. Total cross sections are trusted, new IRMM measurements support a higher elastic cross section, implying that the inelastic cross section should be lowered.

The following benchmarks were analysed to validate the improved Fe-56 evaluated data file:

- IPPE benchmarksfrom ICSBEP –leakage spectra from thick iron spheres with a Cf-252 source in the centre.
- ASPIS-Fe88 benchmark from SINBAD - deep penetration case with a ^{235}U fast fission spectrum (new models developed by B. Kos from JSI under contract with the IAEA).
- IPPE benchmarks from SINBAD – leakage spectra from thick iron spheres with a D-T source in the centre (Analysis model originally developed by A Milocco at JSI).
- LLNL benchmarks - leakage spectra from thick iron spheres with a D-T source in the centre (benchmark models obtained from LANL).
- Oktavian-Fe benchmark from SINBAD - leakage spectra from a thick iron sphere with a D-T source in the centre.
- IPPE iron broomstick benchmarks from ICSBEP with quasi-monoenergetic neutron beams from a p-Li reaction.
- FNS-Fe benchmarks from SINBAD - thick slab ToF transmission spectra from a D-T source at different angles.
- TIARA-Fe benchmarks - 40 MeV and 65 MeV transmission spectra measurements (new models developed by B. Kos from JSI under contract with the IAEA).

Additional benchmarks were analysed, but they did not provide useful information:

- KfK-Fe benchmark from SINBAD – leakage spectra from thick iron spheres with a Cf-252 source in the centre: the results of the analysis by S. Simakov are in contradiction with the similar IPPE benchmarks. This benchmark is rejected.
- NIST-Fe benchmark from SINBAD - leakage spectra from thick iron shells with a ^{252}Cf source: the measured data are too coarse to provide useful information to discriminate between evaluations.
- Illinois-Fe benchmark from SINBAD - leakage spectra from thick iron shells with a ^{252}Cf source: similar problem as with the NIST-Fe benchmark.
- EURACOS benchmark from SINBAD - deep penetration case with a ^{235}U fast fission spectrum: the source spectrum is poorly defined; the measured activation rates without iron in place cannot be reproduced adequately in simulations.
- LSD-RPI benchmark – lead-slowing-down experiment: the statistical scattering of the measured data is too large to discriminate between evaluations.

Some other benchmarks were identified that might be useful for the validation of the iron cross sections:

- NRI & Skoda leakage spectra from thick iron shells with a ^{252}Cf source, ANE 20, 9, (1993), Sajo et al.). It should be noted that new measurements from NRI Rez also exist, but are not available.
- ORNL Broomstick experiments (SINBAD) were not analysed so far.
- Ohio University benchmarks include different cases – e.g. Wenner et al. NSE 170 207 (2012), but the details are not available.
- RPI-Fe quasi-differential cross section measurements – we are waiting for the data to be released.

Problems identified in the CIELO evaluation were largely removed in the current INDEN evaluation, while retaining good performance in the criticality calculations.

INDEN Fe-56 evaluation is a significant candidate for inclusion in a future version of the FENDL library.

A general recommendation is to investigate additional benchmarks suitable for inclusion in SINBAD, but also those benchmarks that are already included in SINBAD where the documentation or models are deficient or missing. The SINBAD meeting is due soon and these issues should ideally be discussed there.

Discussion
S. Simakov demonstrated that the NIST-Fe benchmark can be useful for validation, except at the low energy end, and supports the IPPE measurement. He agrees that the KfK-Fe benchmark should be rejected.

2.8. Ulrich Fischer – Remarks on the use of FENDL-3.1 for IFMIF-DONES (ENS project)

U. Fischer described the IFMIF-DONES neutron source facility developed by EUROfusion within the ENS (Early Neutron Source). The main mission to provide the irradiation data required for the construction of DEMO. The computational tools include the MCUNED code (an extension of MCNPX by UNED, Madrid) for the deuteron transport and the McDelicious code (an extension of MCNP-5/-6 by KIT) for the (d-Li) neutron source generation and the n-γ transport simulations. MCUNED can use deuteron data files as prepared for TENDL-2015 in a dedicated format utilizing a Kalbach-Mann type data representation. A. Koning commented that this TENDL-2015 version requires some special NJOY extensions developed by P. Sauvan at UNED (it is not available but only used by UNED in the ENS project). The McDelicious code uses ad-hoc prepared ENDF/ACE data files for the d + ^{6,7}Li(d,xn) reaction which are provided together with the code. These data files can be also made available to the IAEA/NDS (inquiry by AT). McDelicious is available upon request, MCUNED can be ordered from the NEA Data Bank.

Nuclear data:

FENDL-3.1d is used as the reference neutron cross-section data, FENDL-3.0/A (identical to EAF-2010) for the activation data. An advanced activation data library based on TENDL-2017 is currently prepared within the EUROfusion programme.

Deuteron cross sections are based on TENDL -2015, testing with TENDL-2017 is underway.

For damage calculations, special displacement damage cross sections, prepared for Eurofer and SS-316 steels in DEMO and ENS applications, are used. They are available through the IAEA/NDS website.

For individual elements the recent JEFF-3.3 dpa data library is the recommended data source. These are available form the NEA Data Bank web site for JEFF-3.3.

<u>Discussion/Conclusions:</u>
U. Fischer concluded that major nuclear data improvements are required for the deuteron data libraries, including updated TENDL data and new JENDL deuteron evaluations. These show good agreement with experimental data, as seen in S. Kunieda's presentation. The neutron activation data library needs to be updated by adopting e.g. the new TENDL-2017/EAF type activation library prepared by EUROfusion.

The use of a dedicated FENDL sub-library for dpa data was discussed. This is now accepted as an interim solution before the next major FENDL release (see the discussion above).

C. Konno asked about the impact of cross section data > 20 MeV in O-16. U. Fischer commented that there was little impact for IFMIF-DONES applications but the O-16 evaluation should be updated in FENDL as previously agreed.

M. Fabbri from F4E asked when the EAF format TENDL-2017 library will be available. U. Fischer answered that the library is ready but currently being tested. The release is expected in January 2019.

2.9. Ulrich Fischer – FENDL Quality Assurance: Proposal for V&V procedure

U. Fischer outlined the general V&V definitions making the distinction about technical tools and processes by which simulation credibility is quantified.

With regard to FENDL data V&V he pointed out that this includes: i) data file checking using e. g. ENDF utilities, PREPRO, backward conversions with ACELST (ACE to ENDF) and comparisons to original ENDF data, and ii) comparison of evaluated data against measured cross section data.

With regard to the application of FENDL data, the validation process is performed on the nuclear cross sections in application data files, e.g. ACE, GENDF, with the demonstration that correct simulation results are obtained when comparing to results of integral benchmark experiments.

The previous FENDL-3.0 benchmarking procedure included:

1) Computational benchmarks to check the performance of application data libraries against previous file versions – typically comparing nuclear responses e.g. neutron and photon fluxes, spectra, nuclear heating, gas production, displacement damage.
2) Experimental benchmarks to check the performance of data files against fusion relevant benchmark experiments, e.g. FNS, Tokai-mura, FNG, Frascati.

(There is a detailed report by U. Fischer et al., "Benchmarking of the FENDL-3 neutron cross section data library for fusion applications").

However, the benchmarking was incomplete since testing was done only for some applications, some materials and some specific response. A more systematic approach is required for the future. Therefore, the following V&V procedure is proposed:

*V&V of ENDF & processed data files, including comparisons/cross sections against previous and/or other data file evaluations + 'human inspections'

(A. Trkov agrees to compare against the current TENDL-2017 evaluation and another library in case the FENDL evaluation comes from TENDL. COMPLOT (from PREPRO) can be used to compare with other evaluations. Checking procedures already exist for data processing validation, see for example the specification in the following report: INDC(SEC)-0106).

*Benchmarking of application data files should include, as a minimum requirement, comprehensive computational benchmarks on single isotopes, e.g. in a spherical shell configuration with central 14 MeV neutron source (also higher energies could be considered). Automated scripts can be used for running transport calculations, results processing and visualisations. In addition, specific computational benchmark relevant to shielding (including also bio-shield configurations), tritium breeding, and streaming should be conducted. These could be extended to other nuclear responses of interest e.g. heating, dpa and gas production. 1D benchmarks (as the one developed by M. Sawan, and another one for tritium breeding), and 3D benchmarks using e.g. the 40 degree ITER benchmark model (from 2005) to compare neutron and photon fluxes, TFC nuclear responses, etc. would be valuable. Another 3D benchmark could be performed on DEMO or FNSF for the tritium breeding and other responses.

*Experimental benchmarks – a suite of pure benchmark experiments (single material, simple configuration) and design-oriented benchmark (many materials, complex mock-ups etc.) should be considered.

The following **pure benchmark experiments** can be considered:

Spherical shells with central 14 MeV neutron source: LLNL pulsed sphere experiments (many materials, ToF spectra), IPPE Obninsk (Fe), KfK (Be, Fe), OKTAVIAN (many materials),

2D/3D geometry (typically cylinders or rectangular blocks) with external 14 MeV neutron source: FNS experiments (many materials, ToF and reaction rates), FNG experiments (W, SiC, Cu).

It is stressed that proper documentation of the experiments is necessary, and the quality & suitability needs to be adequate. Preferably the experiments should be available in the SINBAD compilation. A. Trkov mentioned that A. Milocco made a quality assessment of benchmarks experiments in SINBAD, see: https://www.oecd-nea.org/science/wprs/shielding/sinbad/.

Complex geometry experiments: The ITER bulk shield & streaming experiments and the tritium breeding experiments (FNG HCPB and HCLL), previously already used, are to be used, other shielding/streaming experiments (e.g. those from ORNL included in SINBAD) might be considered.

There is a set of TIARA experiments at 40 and 65 MeV neutron energy which should be used to test the high energy applications (E> 20 MeV).

U. Fischer concluded that extended benchmarking is required for improved V&V analyses of (future) FENDL libraries. The recommended approach is to conduct a set of computational benchmarks including single materials, with 1D and 3D benchmarks, a set of experimental benchmarks on single materials, mock-ups, as well as complex shielding and streaming experiments which should be mandatory to be run before a library is released.

3. Discussion

3.1 General Discussion

The IAEA is the custodian of FENDL. IAEA can do V&V of library, include some computational benchmarks for pure materials e.g. look at leakage spectra, perhaps the 1D benchmarks. The burden of work for more complex benchmark comparisons needs to be shared, as practised previously. Efforts should be made to get experimental benchmark data into SINBAD. It has to be agreed what the minimum effort should be and what is 'nice to have'.

A staged testing approach is considered suitable with mandatory stages to identify any issues in the application data files, with 3D modelling e.g. ITER models coming later. E. Polunovskiy commented that ITER Organization (IO) could potentially manage the final testing of 3D models. The ITER benchmark model (2005) could be made available to everybody by the IAEA.

Experimental benchmark discussion

There was some discussion on whether to use e.g. the LLNL pulsed sphere data, and whether it could be made available. There is a meeting coming up in Paris: on ICSBEP/SINBAD. U.Fischer agreed to speak to Dieter Leichtle to raise this issue at that meeting. Wim Haek has performed studies using these data and it was suggested that he could be contacted too.

There was some discussion on the availability of the FNS data that is not available in SINBAD.

Action: C Konno to identify if data from FNS models/data (not already available in SINBAD) are available for the purposes of benchmarks. It is not quite clear whether the data is owned by JAEA or QST which could cause some complexities in releasing the data.

There was some discussion on whether the ORNL 'broomstick' experiments should be included (from 1968). These are transmission experiments to measure the total cross section. The value of the experiments is unknown, but perhaps a task for 2 months would be needed to investigate.

3.2. Other issues that were discussed:

E. Polunovskiy mentioned that ITER was interested in 3 different temperature libraries: 4k for SC coils, 293 K and 400 K (which is the working temperature of the VV). Thermal scattering kernels for cryogenic temperatures were discussed as they are not available. T. Bohm commented that in work examining temperatures greater than room temperature, for example 100 C, that density is the dominant effect with temperature changes. He referred to the following report, which provides more details: Bohm, et. al, "Recent 3-D Neutronics Analysis of ITER Blanket Modules and the Impact of Temperature on Neutronics Modeling for ITER", presented at the XII ITER Neutronics Meeting, 10-12 October 2017, Cadarache, France, ITER documentation report: ITER_D_VLFUEV.

M. Fabbri commented that they did not find any significant temperature differences in their studies. C. Konno commented that the thermal scattering effect is likely to be very small. In conclusion the priority of these libraries was deemed to be 'secondary' by E. Polunovskiy.

Action: EP to provide a list of ITER needs and priorities. (Possible extensions include U-234, Ta-180 and Neon isotopes)

3.3. Discussion on MCNP5 running problems when using the FENDL-3.1d ACE files

MCNP5 is used extensively for ITER calculations, particularly in connection with the UNED D1S patch, which is practically necessary to plot and run the geometrically complex ITER C-model. However, there is an issue with using FENDL-3.1d ACE files with MCNP5.

The Fe-56 file has been re-processed using NJOY-2012.137 and NJOY-2016.44. The two ACE files were sent to M. Fabbri at F4E by DLA during the meeting. These two files will be tested by him using MCNP5 with a simple 1 m radius sphere of Fe-56 and with a 20 MeV point isotropic neutron source at the centre. He will first try to reproduce the issue using the existing FENDL-3.1d library before testing the new ACE file. If the issue appears to be resolved following this test, the full set of isotopes will be reprocessed using this methodology. (Action: M. Fabbri agreed to send the MCNP5 output files to C. Konno and D. Lopez Aldama)

An issue relating to coincident points existing in the following nuclide files was identified at F4E for B-11, Mo-95, Er-162, Er-164 and Er-170. There may be other nuclides with this issue. (Action: source ENDF files are to be checked by A. Trkov)

Discussion
M. Fabbri tried to reproduce the error with FENDL-3.1d on the proposed model problem during the meeting, but the result was negative.

3.4. Concluding discussions

There was an extensive discussion relating to fixing the FENDL-3.1d issue discussed earlier, as outlined in S. Kwon's presentations. A fix for Fe-56 from INDEN already exists, and for other nuclides a number of possible solutions were suggested:

1) Do nothing;
2) Use 22 MeV spectra;
3) Use 22 MeV spectra, rescale the outgoing energy and renormalize;
4) For Fe-56 double differential data <20MeV are included in the file, so interpolation to 20 MeV from neighbouring points would seem to be possible. However, this needs to be checked for other nuclides.
5) Change JENDL-4/HE to law 1;
6) Re-run TENDL formatting with a breakpoint at, for example, 18 MeV and use the spectrum at 20 MeV;
7) Fix TENDL the formatting and replace the HE with new TENDL.

Action: A. Koning to reformat TENDL and include a different break point at, for example, 18 MeV. This is initially to be performed on a single isotope. If the problem is resolved the fix will be repeated for the remaining nuclides (about 60). This is seen as a priority and A. Koning agreed to complete this task this year. The runs will not include covariance data and it therefore is not particularly computational expensive (perhaps a couple of days).

If the fix works, the recommendation is to include this in FENDL-3.2.

3.5. FENDL-3.2 and FENDL-4.0 discussions

It was agreed that the focus is to fix the current issues i.e. 'clean up' FENDL-3.1. It is thought that the current fixes which are needed are significant enough to merit a move to FENDL-3.2. This will create a good reference for an eventual move to FENDL-4.0. The strategy for the preparation of FENDL-4.0 will be decided at the next meeting, which is expected to take place in about 1 years' time.

The expected timeline for the release of FENDL-3.2 is by June 2019. An unofficial pre-release version will be made available for testing as soon as it is ready.

Activation files – the proposal was for TENDL-2017 to be adopted in FENDL-3.2 (neutron, but also deuteron and proton). The JENDL/AD-2017 evaluations (which only go up to 20 MeV) should be included in the benchmark comparisons for consideration in future updates.

There was a discussion about photo-nuclear libraries. There is particular interest from ITER in photo-nuclear interactions in Be (e.g. for cask transfer applications, runaway electron phenomena). There are existing photo-nuclear libraries that can be used by MCNP (la150u, endf7u) and it was proposed to continue with these for the time being. JAEA have a photo-nuclear data library, JENDL/PD-2016, which is available in ENDF-6 format. The JAEA library is still to be processed into ACE files and then tested. Once these are available the library can be considered for future use in a FENDL release, for example in FENDL-4.0.

Consultants' Meeting on the FENDL Library for Fusion Neutronics Calculations

IAEA Headquarters, Vienna, Austria
15 to 18 October 2018
Meeting Room MOE61

Adopted AGENDA

Monday, 15 October

08:30 – 09:00 **Registration** (IAEA Registration desk, Gate 1)

09:00 - 09:30 **Opening Session**

Welcoming address – Arjan Koning, SH/NDS
Introduction – A. Trkov
Election of Chairman and Rapporteur
Adoption of Agenda
Administrative matters

09:30 - 12:30 **Presentations by participants** (~ 30 min' each)

1. *Processing nuclear data for FENDL-2.1 and FENDL-3.1d.*, D. Lopez Aldama
2. *The Impact of ENDF/B-VIII.0 and FENDL-3.1d Data on Fusion Neutronics Calculations*, T. Bohm
3. *New comments on data below 20 MeV in FENDL-3.1d*, Ch. Konno

12:30 – 14:00 ***Lunch***

14:00 – 17:30 **Presentations by participants** (cont'd)

4. *Significant comments on data above 20MeV in FENDL-3.1d*, S. Kwon
5. *1) Remarks on the use of FENDL-3.1 for IFMIF-DONES (ENS project), 2) FENDL Quality Assurance: Proposal for a V&V procedure*, U. Fischer
6. *Recent evaluation/benchmark works in the JENDL project relevant to FENDL*, S. Kunieda
7. *Nuclear data validation efforts*, L. Packer
8. *INDEN (Post-CIELO) ^{56}Fe Evaluation*, A. Trkov

Coffee breaks as needed

Tuesday, 16 October

09:00 - 12:30 **Round table discussion**

12:30 – 14:00 *Lunch*

14:00 – 17:30 **Round table discussion (cont'd)**

Discussion on the presentations

Coffe breaks as needed

19:00 ***Dinner at a restaurant (see separate information sheet)***

Wednesday, 17 October

09:00 - 12:30 **Round table discussion** (cont'd)

Discussion on the presentations

12:30 – 14:00 *Lunch*

14:00 – 17:30 **Round table discussion** (cont'd)

Drafting of the Summary Report

Coffee breaks as needed

Thursday, 18 October

09:00 - 16:00 **Drafting of the summary report** (cont'd)

Finalisation of the Summary Report and Action List

16:00 **Closing of the meeting**

Coffee break(s) and lunch in between

IAEA
International Atomic Energy Agency
Atoms for Peace and Development

Consultancy Meeting on the

FENDL Library for Fusion Neutronics Calculations

15 to 18 October 2018
IAEA, Vienna

List of Participants

CUBA

Daniel LOPEZ ALDAMA
Agency of Nuclear Energy and
Advanced Technologies (AENTA)
Calle 20 no. 4109e/41 y 47
Miramar Playa
La Habana
E-mail: aldama@aenta.cu

GERMANY

Ulrich FISCHER
Karlsruher Institut für Technologie (KIT)
Institut für Neutronenphysik und Reaktortechnik (INR)
Postfach 3640
76021 Karlsruhe
E-mail: ulrich.fischer@irs.fzk.de

JAPAN

Satoshi KUNIEDA
Japan Atomic Energy Agency (JAEA)
Nuclear Data Center
Shirakata-Shirane 2-4
Tokai-mura, Naka-gun
Ibaraki-ken 319-1195
E-mail: kunieda.satoshi@jaea.go.jp

Chikara KONNO
Nuclear Data and Reactor Engineering Division
Nuclear Science and Engineering Center
Japan Atomic Energy Agency
Shirakata 2-4
Tokai-mura, Naka-gun
319-1195 Ibaraki-ken
E-mail: konno.chikara@jaea.go.jp

Saerom KWON
Advanced Fusion Neutron Source Design Gr.
Department of Fusion Reactor Materials Research
Rokkasyo Fusion Institute
Fusion Energy Research and Development Directorate
National Institutes for Quantum and Radiological Science and Technology
2-166 Omotedate, Obuchi, Rokkasyo-mura, Kamikita-gun, Aomori 039-3212
E-mail: kwon.saerom@qst.go.jp

UNITED KINGDOM

Lee PACKER
UK Atomic Energy Authority
D3 Culham Science Centre
Abingdon OX14 3DB
E-mail: lee.packer@ukaea.uk

UNITED STATES

Tim BOHM
University of Wisconsin-Madison
Engineering Research Building
1500 Engineering Dr
Madison WI 53706
E-mail: tim.bohm@wisc.edu

ITER Organization

Eduard POLUNOVSKIY
ITER Organization
Route de Vinon-sur-Verdon-CS90046
13067 St Paul lez Durance Cedex
Email : Eduard.Polunovskiy@iter.org

Remote Participation

Marco FABBRI
Technical Support Services / ITER Department
Josep Pla 2
Torres Diagonal Litoral B3 02/20
08019 Barcelona
Spain
E-mail: marco.fabbri@f4e.europa.eu

IAEA

Andrej TRKOV
Scientific Secretary
Tel. +43-1-2600 21712
E-mail : a.trkov@iaea.org

Arjan KONING
E-mail: a.koning@iaea.org

Daichi IMAZATO
E-mail: d.imazato@iaea.org

Takanari FUKUDA
E-mail: t.fukuda@iaea.org

All:
International Atomic Energy Agency
NAPC/ NDS
Wagramer Strasse 5
1400 Vienna
Austria

Presentations

#	Author	Title	Link
1	D. Lopez Aldama	Processing nuclear data for FENDL-2.1 and FENDL-3.1d	PDF
2	T. Bohm et al.	The Impact of ENDF/B-VIII.0 and FENDL-3.1d on Fusion Neutronics Calculations	PDF
3	U. Fischer	Remarks on the Use of FENDL-3.1 for IFMIF-DONES (ENS project)	PDF
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Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna, Austria

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: http://nds.iaea.org