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FENDL Library for Fusion Neutronics Calculations
Summary Report from the Technical Meeting
IAEA Headquarters
2-5 September 2019

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October 2019

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ABSTRACT

The status of the FENDL-3.1 library was reviewed in view of the recommendations from the previous meeting in 2018. It was decided to adopt the IAEA INDEN evaluation for ^{56}Fe and a modified ^{16}O evaluation provided by QST and JAEA, Japan. The Activation library will be adopted from TENDL-2017, except for evaluations that are included in the IRDFF-II library; for incident charged particles, preference will be given to the evaluations in the medical isotope cross section library. With the proposed changes the library FENDL-3.2 for fusion neutronics calculations will be released from the IAEA.

October 2019

Contents

1. Introduction

A. Trkov, Scientific Secretary of the meeting welcomed the participants of the Technical Meeting. He proposed M. Sawan as Chairman and D. Leichtle as Rapporteur of the Technical Meeting, respectively. The participants raised no objections.

A. Koning, Head of IAEA Nuclear Data Section, gave a welcome address, where he commended the current efforts on maintenance of the FENDL library addressing in particular feedback from integral testing. In this way, several improvements have been achieved.

R. Capote stressed the importance to deliver a new release, namely FENDL-3.2, for the fusion community. The current meeting has the objective to advise IAEA-NDS on the open issues relevant for the release and to reflect on users' needs.

In the technical introduction to the meeting, A. Trkov confirmed that several actions of the previous meeting have been successfully addressed, while a few are still pending. This includes the negative KERMA from p-tables, which will be addressed in C. Konno's contribution to the meeting. Regarding issues with using FENDL-3.1d in MCNP5, as reported by M. Fabbri, this has not been confirmed from testing at IAEA-NDS. The request of E. Polunovskiy (see also M. Loughlin's presentation in the current meeting) for neutron transport libraries for several nuclides has not yet been assessed. He also recalled that benchmarking by JAEA/QST and IAEA-NDS has shown some contradicting results, which need clarifications.

2. Summary of presentations by participants

2.1 S. Kwon (QST, Japan), Benchmark test for next FENDL

The following four items were presented by S. Kwon:

(1) INDEN ^{56}Fe benchmark test with QST/TIARA iron shielding experiments for FENDL-3.2

(2) Benchmark test with QST/TIARA concrete shielding experiments for new ^{16}O data

(3) Problems on neutron production data of deuteron-induced files in TENDL-2017

(4) New ^{56}Fe benchmark test with QST/TIARA iron shielding experiments for next TENDL, TENDL-2019

<u>(1) INDEN ^{56}Fe benchmark test with QST/TIARA iron shielding experiments for FENDL-3.2</u>

At the last FENDL meeting, Dr. Trkov proposed that INDEN ^{56}Fe would be a candidate of FENDL-3.2. However, it was not clear whether INDEN ^{56}Fe was better than FENDL-3.1d ^{56}Fe. Thus, we carried out benchmark tests of INDEN ^{56}Fe with the QST/TIARA iron shielding experiments. In the iron experiment with 40 MeV neutrons, the calculated neutron fluxes using INDEN ^{56}Fe agree well with the experimental ones both in the continuous region from 10 to 35 MeV and the peak region from 35 to 45 MeV. In the iron experiment with 65 MeV neutrons, however, the calculated neutron fluxes using INDEN ^{56}Fe underestimate the experimental ones both in the continuous region from 10 to 60 MeV and the peak region from 60 to 70 MeV. It is not affirmed that INDEN ^{56}Fe is better than FENDL-3.1d ^{56}Fe. We propose that FENDL-3.2 should adopt FENDL-3.1d ^{56}Fe, where only the secondary neutron spectrum data at 20MeV in mt=5 are revised as we had proposed at the last FENDL meeting. We need to check the version of INDEN ^{56}Fe; we used "fe56e80X29r2" in the analyses, while Dr. Trkov showed the version “fe56e80X29r34” in his introduction slide. We are not sure how different are the two files and whether the changes are only minor.

Discussion

- The performance of INDEN file in resonance region and up to 43 MeV is excellent. This has been shown in other benchmarks.
- If the neutron spectrum of the facility has significant contributions above 50 MeV, users are advised to check their results against FENDL-3.1d or JENDL-4.0/HE.

Decision

- FENDL-3.2 will adopt ^{56}Fe file from INDEN, version “X29r34”.

Actions

- A. Trkov: to compare INDEN ^{56}Fe file versions (r2 vs. r34) and upload to meeting website.

(2) Benchmark test with QST/TIARA concrete shielding experiments for new ^{16}O data

As one of the actions at the last FENDL meeting, Dr. Kunieda prepared new ^{16}O data for the next FENDL library. The ^{16}O data of FENDL-3.1d was taken from ENDF/B-VII. Dr. Kunieda replaced the ^{16}O data of FENDL-3.1d with those of JENDL-4.0/HE over 30MeV, where the upper energy limit was changed from 200 to 150 MeV (FENDL-3 new1). As a benchmark test of the new ^{16}O data, we analyzed the QST/TIARA concrete shielding experiments. In the concrete experiment with 40 MeV neutrons, although the calculated neutron flux with FENDL-3 new1 still overestimates the experimental one in the continuous region from 10 to 35 MeV, the overestimation is improved a little. The calculated neutron flux with FENDL-3 new1 agrees well with the experimental one in the peak region from 35 to 45 MeV. In the concrete experiment with 65 MeV neutrons, the calculated neutron flux with FENDL-3 new1 agrees well with the experimental one in the continuous region from 10 to 60 MeV. The calculated neutron flux with FENDL-3 new1 still overestimates the experimental one in the peak region from 60 to 70 MeV, even though the overestimation is improved a little. In addition, in order to clarify an impact of data between 20 and 30 MeV, we modified the Kunieda’s ^{16}O data; the data above 20 MeV were replaced with those in JENDL-4.0/HE (FENDL-3 new2). We confirmed the impact of data between 20 and 30 MeV and figured out that the data between 20 and 30 MeV in FENDL-3.1d should also be replaced with those in JENDL-4.0/HE. We affirmed that the two ^{16}O data are better than FENDL-3.1d ^{16}O data.

Decision

- will adopt ^{16}O-file provided by C. Konno/S. Kwon (S. Kunieda).

Actions

- S. Kwon/C. Konno: to contact S. Kunieda for his evaluation; to send new ^{16}O-file (“new2”).

(3) Problems on neutron production data of deuteron-induced files in TENDL-2017

Charged particles-induced files (p, d, t, He3, α up to 200 MeV) in TENDL-2017 was released on Dec. 30, 2017. A nuclide has 3 kinds of ENDF files, the TENDF file, Special ENDF file and Another special ENDF file. All files are based on the same TALYS calculation, but they differ in ENDF representation. The so-called “Another special ENDF file” has all reaction cross section lumped into MT5, with all outgoing particle distributions in MF6. There is only one official ACE file of the TENDF file in TENDL-2017. Up to TENDL-2015, the TENDL libraries have only the file corresponding to Another special ENDF file of TENDL-2017. Eventually, the 3 files must be consistent. But K.L. Paaren et al. reported that the TENDF file of ^{9}Be in the α-induced files of TENDL-2017 produced strange neutron spectra, while Another special ENDF file produced reasonable neutron spectra. Thus, we investigated whether the deuteron-induced files in TENDL-2017 have the similar problem to the α-induced files or not. In order to investigate the three ENDF files of ^{9}Be in TENDL-2017, we made ACE files of the TENDF file, Special ENDF file and Another special ENDF file of ^{9}Be using NJOY2016.49 modified for a bug related to mt=11. Then we extracted and compared neutron production cross sections and secondary neutron energy distributions from NJOY outputs of the three ENDF files for no ACE format information of (d,xn) reactions. We found out that neutron production cross section above 30 MeV in Special ENDF file differs markedly from those in the other ENDF files and produces smaller neutron fluxes for deuteron above 30 MeV. We also found wrong secondary neutron energy distribution data in the TENDF file and/or special ENDF file, which caused broad peak near 30 keV and small peak near 30 MeV in calculated neutron spectra. Another special ENDF file seems to be physically correct in the three ENDF files. The same problems probably occur in other nuclei of TENDL-2017. The deuteron-induced ENDF and ACE files in TENDL-2017 should be revised based on our study.

Discussion

- Use of TENDL-2017 charged particle general purpose files for transport is only possible via "another special ENDF format" (lumped MT5 only), as labelled on TENDL-2017 webpage (https://tendl.web.psi.ch/tendl_2017/tendl2017.html).
- TENDL-2017 charged-particle activation files are available.

Decision and recommendation

- FENDL-3.2 charged particle induced activation files will adopt TENDL-2017 (explicit channels) with the following recommendation:
- Where data in the ENDF-file from incident charged-particle medical isotope cross section data (https://www-nds.iaea.org/medical/) are available, they shall be taken in preference to TENDL-2017.

Actions

- A. Trkov: to produce ENDF-file from incident charged-particle medical isotope cross section data.
- R. Capote/J-C. Sublet: to assess the feasibility of merging TENDL-2017 and medical isotope cross section data in a single FENDL activation library.

(4) New ^{56}Fe benchmark test with QST/TIARA iron shielding experiments for next TENDL, TENDL-2019

We pointed out strange data in TENDL-2017 at the last FENDL meeting (14-18 Oct. 2018).

In TENDL-2017, 2595 nuclei had incorrect secondary neutron spectrum data at 30 MeV (in 2807 data). Dr. Koning prepared new ^{56}Fe data for TENDL-2019 where a format error at 30 MeV was corrected. Thus, we carried out a benchmark test of the new ^{56}Fe data with the QST/TIARA iron shielding experiments. The incorrect secondary neutron energy spectrum data in ^{56}Fe of TENDL-2017 are corrected in the new ^{56}Fe data. There were no strange peaks around 30 MeV in the calculated neutron spectra with the new ^{56}Fe for the experiments with 40 and 65 MeV neutrons. The analyses of QST/TIARA iron shielding experiments affirm that the new ^{56}Fe data are better than those in TENDL-2017, although the new ^{56}Fe data are not "perfect" (The calculated neutron fluxes with the new ^{56}Fe underestimate the experimental ones in the peak region from 60 to 70 MeV). The incorrect secondary neutron energy spectrum data in ^{54}Fe and ^{58}Fe of TENDL-2017 have to be corrected. We checked the effect of the other iron nuclei data. Although the effect was not so large, further study should be performed including the improved data for the other iron nuclei. The new ^{56}Fe data is also a candidate for the next FENDL file.

2.2 L. Leal, Angular Data from Resonance Parameters, is it a viable option?

The presentation reports on the resolved resonance evaluation including double differential experimental data for better resonance spin determination. The formalism developed by Blatt-Biedenharn (BB) relates the angular dependent cross section with the collision matrix (scattering matrix). Nuclear data evaluation codes such as CONRAD and SAMMY, for instance, are based in the R-matrix formalism. In addition, these codes incorporate the BB methodology, then permitting the evaluation of double differential cross section in the resolved resonance region. While the evaluation can be done the question to be addressed is whether experimental data with reasonable resolution exist or can be measured to allow evaluator to explore the determination of resonance parameters which can reproduce the usual cross sections such as total, capture, fission as well as the angular dependence of the scattering cross section whether elastic and/or inelastic. A simple example based on the SAMMY fitting of the double differential elastic scattering cross section ^{56}Fe measured by Perey at the Oak Ridge Electron Linear Accelerator was presented. The data were fitted with a single set of resonance parameters up to 840 keV for six angles, namely 39, 55, 90, 120, 140, and 160 degrees. It was not clear for the presenter (Leal) that the question raised whether the procedure for fitting angular data in the resonance region is a viable option if consistent and good resolution data are not available.

Discussion

- Apparently, the detailed representation for angular data for most applications is not needed. However, analysis of angle-dependent TOF data for fitting the resonance parameter is important for the consistency of angular distributions with associated resonance parameters.
- Users can reconstruct detailed angular distributions from resonance parameters, if needed. Usually, MF4 contains resolution-broadened angular distribution, which are sufficient for most practical applications.

2.3 A. Ignatyuk, Test of the FENDL-3.1 activation data against the revised experimental data for the charged-particle induced reactions

Considerable amount of experimental data on the charged-particle induced reactions was obtained during the last decade and many of them were revised in the under the Medical CRP in 2012-2018. The available experimental data were compared with the FENDL-3.0/A (TENDL-2011), TENDL-2015, and TENDL-2017 libraries, exhibiting for many cases significant disagreements in the magnitude and shape of the corresponding excitation functions.

A revision of available data for about 150 reactions was performed on the basis of the “unrecognized-error estimation method” developed at IPPE. Along with a consistent consideration of statistical errors of experimental data the method allows to determine some systematic uncertainties, usually underestimated by the authors of data, and to establish also some implicit correlations of data. An account of systematic uncertainties is an important feature of the method.

The recommended cross sections together with evaluated uncertainties are available now on the web page of the IAEA medical portal www-nds.iaea.org/medportal. These data are important for existing and potential nuclear medicine applications, and they may also have been useful for the fusion projects to improve the charged-particle activation library.

Actions

- See previous action above on producing ENDF files of medical isotope cross section data.
- J-C. Sublet: to compare (d,p)-reactions in TENDL-2017 with FENDL3.0.

2.4 C. Konno, Follow-up from previous FENDL meeting

(1) INDEN ^{56}Fe benchmark tests with JAEA/FNS iron experiments for next FENDL

At the last FENDL meeting, Dr. Trkov proposed that INDEN ^{56}Fe would be a candidate of the next FENDL. However, it was not clear whether INDEN ^{56}Fe was better than FENDL-3.1d ^{56}Fe. Thus, we carried out benchmark tests of INDEN ^{56}Fe with the JAEA/FNS iron experiments. JAEA/FNS iron experiments consist of two experiments. One is a TOF experiment, where angular neutron leakage spectra above 100 keV from a cylindrical iron slab were measured with the TOF method, and the other is an in-situ experiment, where neutron spectra and reaction rates were measured inside a large cylindrical iron slab. As a result, the differences between the calculation results with INDEN ^{56}Fe and FENDL-3.1d ^{56}Fe were not so large. We propose that the next FENDL adopts FENDL-3.1d ^{56}Fe, where only the secondary neutron spectrum data at 20 MeV in mt=5 are revised. We need to check the version of INDEN ^{56}Fe. We used “fe56e80X29r2” in the analyses, while Dr. Trkov showed the version of “fe56e80X29r34” in his introduction slide. We are not sure how different are the two files and whether the changes are only minor.

Discussion

- Contrary to the findings of the presentation, several benchmark exercises have demonstrated excellent performance of INDEN file.

Actions

- C. Konno: to test KERMA for INDEN ^{56}Fe.
- C. Konno: to provide JAEA/QST tools for ACE data interrogation to Andrej.

(2) Re-investigation on p-tables in ACE file of FENDL-3.1d

i) A new solution for negative p-tables of heating number

The reason for the negative p-tables of heating number is that the partial KERMA of the capture reaction is calculated with the energy-balance method, while the total KERMA is calculated with the kinematics method. Thus, we modified NJOY so as to calculate the partial KERMAs of elastic scattering, fission and capture with the kinematics method as well as the total KERMA. Then positive p-tables of heating number were obtained.

ii) p-tables of heating number in official ACE files of other nuclear data libraries

We examined the p-tables of the heating number in the official ACE files of JENDL-4.0, ENDF/B-VIII.0, JEFF-3.3 and TENDL-2017.

- JENDL-4.0: no p-tables of 130 nuclei include negative p-tables of heating number
- ENDF/B-VIII.: p-tables of heating number are average heating number or 1.0.
- JEFF-3.3: negative p-tables for 22 nuclei
- TENDL-2017: all p-tables of heating number are 0.0.

iii) Comment on the IAEA method

At the last FENDL meeting, IAEA decided just to modify p-tables of heating number in the ACE file to 1.0 or average heating numbers without our old method, because our old method omits partial KERMAs. However, this decision is not adequate, because partial KERMAs are calculated with the energy balance method; the ACE file of FENDL-3.1d is no problem because it includes no partial KERMAs, but the MATXS file of FENDL-3.1d includes wrong partial KERMAs and the energy balance is broken. We recommend IAEA to use our new method and revise the ACE and MATXS files of FENDL-3.1d if IAEA wants to leave partial KERMAs in the MATXS file.

Discussion

- JAEA used modified HEATR module of NJOY2016 for the recommended processing.
- Traditionally, FENDL in ENDF is released first, processed files follow. This applies for FENDL-3.2 as well. The present issue affects processing of the ENDF (KERMA) only.

Actions

- C. Konno: to provide modified NJOY-HEATR module to FENDL.
- A. Trkov/J-C. Sublet: to assess the impact of HEATR modifications from JAEA.

(3) Revised ^{40}K data

At the last FENDL meeting, we pointed out that gamma yield and energy distribution data of proton, alpha, residual nucleus and gamma of (n,p) and (n,γ) reactions in ^{39}K of FENDL-3.1d are incorrect, which causes incorrect KERMA and damage energy data. As one of the actions in the meeting, we investigated whether other nuclei have the similar problem to ^{39}K. Then we specified that only ^{40}K had the same problem with ^{39}K. The ^{39}K and ^{40}K data of FENDL-3.1d should be revised based on our study.

Actions

- C. Konno: to send modified $^{39/40}$K ENDF files to A. Trkov.
- A. Trkov: to assess modified files and adopt them for FENDL-3.2.

2.5 S. Nakayama, Introduction of a computational code for deuteron-induced reactions and development plan of deuteron nuclear data files

S. Nakayama introduced DEURACS, which is the code system for calculating the deuteron-induced reaction cross sections. The weakly-bound nature of the deuteron is taken into account explicitly in DEURACS, and it consists of several calculation codes based on theoretical models to describe respective reaction mechanisms that are characteristic of deuteron-induced reactions. The results of double-differential cross sections (DDXs) for (d,xn) reactions on ^{nat}Li, ^{9}Be, and ^{12}C targets were presented. DEURACS reproduced the experimental data better than TENDL-2017. To calculate neutron yield from thick target, database for the PHITS code were developed based on the DEURACS calculation. The DDXs for the emission of each particle (n, p, d, t, 3He, and α) and γ-ray were compiled in the format of “Frag Data” uniquely defined in PHITS. The results of the PHITS simulation using the database reproduced very well the experimental neutron yields from thick ^{nat}Li, ^{9}Be and ^{12}C targets. Development of ENDF-6 format file based on the DEURACS calculation are planned. The file for $^{6/7}$Li, ^{9}Be, and ^{12}C will be made by the end of 2019.

Discussion

- The methodology has been adopted on light-mass nuclides. It is applicable up to medium-mass nuclides (e.g. structural materials).
- It is suggested to adopt the available deuteron files for FENDL-3.2. However, due to schedule of FENDL-3.2 release, it is likely that the new files (see actions) will not be available for adoption in FENDL-3.2.

Decisions

- **FENDL-3.2 will adopt deuteron transport files from S. Nakayama, if available in due course.**

Actions

- S. Nakayama: to provide deuteron files for $^{6/7}$Li to FENDL, when available.
- S. Nakayama: to provide deuteron files for ^{9}Be and ^{12}C to FENDL, when available.
- A. Trkov/R. Capote: to check status and possibility to adopt deuteron files for FENDL-3.2 (if received by 12/2019).

2.6 M. Sawan, UW-Madison Neutronics Activities to support FENDL

M. Sawan presented the results of calculations performed by T. Bohm at the University of Wisconsin-Madison in response of recommendations and action items identified in the meeting last year.

An issue identified last year was that there is likely a deficiency in the cross-section data for the structural elements in ENDF/B-VIII.0. These include ^{56}Fe, ^{58}Ni, ^{60}Ni, ^{52}Cr, ^{53}Cr, ^{63}Cu, and ^{65}Cu. In order to verify whether these isotopes were the cause of the large differences observed in results for the ITER 1-D computational benchmark, an isotope substitution study was performed. The ITER 1-D calculation was repeated with ENDF/B-VIII.0 with the cross-section data for these isotopes replaced by those from FENDL-3.1d. Replacing the data for ^{56}Fe only resulted in neutron fluxes that get closer to those of FENDL-3.1d until deep in the FW/Blanket Shield and in the VV (Inconel shells) and TF coil (significant Cu content). This implies that ^{56}Fe ENDF/B-VIII.0 data contributes to most of the observed differences. When data for ^{56}Fe, ^{58}Ni, and ^{60}Ni were replaced, the results became closer to those of FENDL-3.1d, particularly close to the Inconel vacuum vessel shells. When all the isotopes of concern were replaced, we see neutron fluxes that closely match those of FENDL-3.1d both near the FW Cu layer and the TF coil which has significant Cu content. This implied that the ENDF/B-VIII.0 data for ^{56}Fe, Cu, Ni, and Cr are the major contributors to the differences observed between ENDF/B-VIII.0 and FENDL-3.1d. The ^{56}Fe INDEN data (fe56e80X29r34) was used in place of ^{56}Fe ENDF/B-VIII.0, the results were found to more closely match those of FENDL-2.1 but still has a similar shape as that with ENDF/B-VIII.0. This implies the effect of data for Cu, Ni, and Cr that were not modified. We need to assess if ENDF/B-VIII.0 data for these elements can be updated. If such updates are produced, calculations will be repeated with them (T. Bohm).

Discussion

- Benchmark exhibits importance of several materials to nuclear responses (^{56}Fe, Cu, Cr, Ni)
- Changes at copper locations in the models indicate the need to check the quality of Cu evaluations.
- Cu evaluations from ENDF-B/VIII, JEFF3.3 and JENDL-4.0/HE are candidates to be tested.
- Based on the benchmarking outcome (see actions) the $^{63/65}$Cu files might be updated.
- Impact of Ni is high but that of Cr is rather low.

Actions

- S. Kwon: To perform FNS Cu benchmarking
- C. Konno: To contact M. Angelone for FNG Cu benchmarking; if not available to perform the benchmarking.
- A. Trkov: To perform criticality benchmarks for Cu data (for JENDL-4.0/HE).
- A. Trkov: To decide on which Cu evaluation to be adopted for FENDL-3.2.

An MCNP model of the ^{252}Cf source in iron sphere benchmark was produced. The source spectrum provided in the Sajo paper was used in preliminary calculations. However, it was pointed out that this spectrum is not representative of the ^{252}Cf spectrum and that the standard spectrum from the dosimetry file should be used (T. Bohm). The reported preliminary results for the total neutron flux at 1m from the source showed similar differences between the libraries as found with the ITER 1-D benchmark calculation with FENDL-3.1d resulting in the largest flux. The spectrum was the hardest with FENDL-3.1d and the softest with ENDF/B-VIII.0.

Discussion

- The source data used in the benchmark should come from the standard ^{252}Cf (bare) source (from ENDF/B-VIII or IRDFF-II; IAEA-NDS can provide the spectrum on request). Encapsulation of the source is in the MCNP model.
- Other ^{252}Cf on ^{56}Fe benchmarks (spheres, shells) are available.

Actions

- T. Bohm: to repeat the calculations using the standard ^{252}Cf source from IRDFF-II.

As part of a verification suite for FENDL, a 1-D computational benchmark that included breeding material is needed. A 1-D simplified model of the US Fusion Nuclear Science Facility (FNSF) will be created (T. Bohm). Preliminary description of the model was presented. The model will be completed and documented with detailed specifications of the radial build and material composition used in each cell (T. Bohm).

Actions

- T. Bohm: to provide model and documentation of 1D-FNSF to IAEA.

2.7 M. Fabbri, A test suite for fusion libraries

FENDL libraries are the reference nuclear data libraries for the ITER project. Developed under the auspices of the IAEA Nuclear Data Section FENDL provides a dedicated data library with the aim to satisfy the needs of the fusion technology and in particular of the ITER project. The libraries are periodically updated in order to improve and/or correct data or to expand the range of applications. These updates require systematic and extensive V&V, fulfilling rigorous quality assurance requirements. The last FENDL consultants' meeting, dated winter 2018, highlighted the need for a standardized, automated and exhaustive V&V procedure covering all the responses of interest (e.g. flux, heating, gas production, dpa, SDDR, etc. …). Such a test suite would help in anticipating possible problems, spotting missing and/or inconsistent data, and estimating the impact of new releases over the different responses.

Therefore, F4E proposes to design, set-up and develop a FENDL test suite open source tool, which should be composed of three main and independent branches:

- The computational benchmarks

- The experimental benchmarks
- The quality checks

The design of specific tests to standardize the comparison of responses (e.g. 1D Tritium Breeding benchmark) is also envisaged. The application of the V&V, at least partial, to the last version of FENDL available is expected.

Fusion for Energy (F4E) is leading the efforts and coordinating the test suite project, which is strongly encouraged by the IAEA. Therefore, the task(s) to be performed by the partner will be carried out in close collaboration with F4E and IAEA, who will provide expert support and guidance for the tool development.

Taking advantage of the work previously carried out on FENDL3.0 and the SINBAD database, the estimated effort is around 1 ppy. Staged development approach with intermediate exercise is foreseen with a first beta release by summer 2020.

Discussion

- 3D-computational benchmarks do not require geometry models in full details. It is proposed to design specifically a 3D benchmark model appropriate to highlight aspects of 3D-analysis, such as the relative importance of streaming and bulk shielding.
- For ITER, it is proposed to use the available C-lite model with a set of standard tallies (flux, heating). TBM models will be integrated. Tallies should be amended by dpa and gas production responses. Global weight window mesh will be provided as well.
- Updated application libraries for transport will be available in short term after potential updates of the basic transport data. This will allow to perform the proposed V&V.
- F4E effort to develop tools and methods for FENDL V&V is appreciated by the Fusion community.

Actions

- A. Trkov: to setup a repository for computational benchmark files (models, inputs, specification, etc.)
- E. Polunovskiy/M. Fabbri: to prepare the ITER C-lite computational benchmark input; to provide it to the IAEA.
- D. Leichtle: to check availability of previous (simple) DONES facility model for inclusion in the computational benchmark repository.
- D. Leichtle: to check availability of 1D-DEMO model (with breeding blanket options) for inclusion in the computational benchmark repository.

2.8 D. Leichtle, Considerations on V&V needs for FENDL data and application

D. Leichtle presented further considerations on V&V of FENDL following U. Fischer’s talk at the Consultants’ Meeting in 2018. He pointed out the strong links to M. Fabbri’s presentation on a test suite for nuclear data libraries.

Fusion nuclear analysis requires a comprehensive and strong V&V along the full analysis workflow. Nuclear data (like FENDL) is a key generic input data and thus requires a specific V&V for its quality assurance. Despite the international reputation of FENDL, it is currently accepted as reference library only for the ITER project. To promote its status as a fusion reference it is suggested to address the aspects of full and complete libraries with a current emphasis on further enhancements of covariance data and special production and energy release (including damage) cross section data (application libraries).

The objectives of V&V of the processed data are proposed, and respective needs are elaborated. To measure and judge the V&V status, specific suggestions for metrics and acceptance criteria are presented separately for verification by computational benchmarks and validation by experimental benchmarks. In all cases, reasonable estimations of related uncertainties in the benchmark calculations (and in the integral experiments) need to be accounted for. Validation is commonly done in a generic fashion (i.e. for a range of fusion applications), which is acceptable for the FENDL release. Project-specific acceptance criteria need to be defined and applied in the validation exercises.

It is recommended to enhance the V&V procedures of the processed FENDL data. Documentation from processing and the V&V are important project records. FENDL's international standing can be further strengthened by a formalized and internationally recognized V&V framework.

Discussion

- Nuclear data related uncertainties in fusion neutronics should be taken into account. This has rarely been done in the past, but its importance has been recently highlighted by ITER.
- For ITER, nuclear data related uncertainties are not expected to be design drivers.
- Currently, there is very little uncertainty information available in the FENDL transport data. It is requested to address this topic in future FENDL releases by provision of full covariance information.
- It has been suggested to apply "tolerance criteria" on verification cases rather than strict "acceptance criteria".
- WPEC SG47 work is ongoing on SINBAD development on benchmark test cases. It was suggested to contact I. Kodeli.

Actions

- M. Fabbri: to contact I. Kodeli and OECD/NEA (M. Fleming) concerning synergies with WPEC SG47.
- M. Fabbri/D. Leichtle: to outline a document on V&V procedures for FENDL.

2.9 T. Eade, UKAEA Experiences with FENDL

Tim Eade presented a brief overview of the benchmarking work being carried out at the UKAEA. Over the past couple of years, the UKAEA have been involved in a number of benchmarking activities using the FENDL transport and activation libraries. These included the decay heat benchmarking work presented by L. Packer at the FENDL meeting in 2018. T. Eade reiterated that the Indium TENDL-2017 cross section requires updating as the decay heat is currently predicted incorrectly. This may be due to misattribution of cross section to the different isomers. It is important that these are correct as the ^{115}In(n,n')^{115m}In reaction is a key diagnostic reaction in fusion.

UKAEA have also been involved in the JET shutdown dose rate benchmark. The calculations used FENDL transport libraries and EAF2010 activation data – although activation calculations with FISPACT-II and TENDL-2017 are currently under way. Considering the complexity of the geometry and uncertainties in the materials a reasonable agreement has been made between calculation and experiment.

In collaboration with ENEA, the UKAEA have also been involved in a water activation benchmark. This aimed at assessing the activation of water moving though a pipe system while under irradiation at ENEA's FNG. This is of particular importance to the ITER cooling water systems. The FENDL3.1-d cross sections have been used for all neutron transport calculations. The ^{16}O(n,p)^{16}N and ^{17}O(n,p)^{17}N been compared to other libraries in order to calculate the reaction rates. Although the calculations are yet to be finalized promising C/E values of between 0.8 and 0.9 have been achieved. Results from this benchmarking activity will be presented at the upcoming ISFNT14 conference.

The UKAEA are also involved in a EURO fusion task looking at the validation and verification of the SERPENT 2 transport code. During one of the benchmarking exercises, it was noticed that while using JEFF-3.3, SERPENT 2 was reporting negative heating values for Tungsten – this was subsequently found to be due to negative average heating values in the JEFF-3.3 nuclear data library. UKAEA therefore wrote an automated script to check for negative values in the ACE files. This was applied to the FENDL-3.1d library. It was found that 4 DPA reactions (^{10}B, ^{32}S, ^{160}Gd, ^{176}Hf) and 5 Average Heating Numbers (^{32}S, ^{114}Cd, ^{116}Cd, ^{160}Gd, ^{176}Hf) had negative values. All of these were found around 20 MeV. These negative values were shown to make MCNP and SERPENT 2 produce differing nuclear heating results in the region of 20 MeV. Although these values are unlikely to impact fusion relevant calculations for ITER etc, they may have an impact if used for accelerator driven systems. It is hoped that the nuclear heating and DPA values should be corrected in subsequent versions of the FENDL library.

Discussion

- It is recommended to use IRDFF-II for $^{115}In(n,n')^{115m}In$ reaction rate calculations.
- From the simulation of the water activation experiment at FNG, Frascati, using different libraries a factor 5 difference for the $^{17}O(n,p)^{17}N$ production is observed. The experiment is expected to provide confidence on the best data to use.
- The ^{16}O evaluation, that came out of the CIELO project (adopted by ENDF/B-VIII), has ca. 50 % higher absorption in (n,α) in the region 3-8 MeV. This will affect neutron flux behind water-cooled shields. Use of FENDL-3.2 will give conservative shielding estimates.
- JAEA proposes to fix dpa problems as reported here and in the previous meeting.

Actions

- T. Eade: to provide data of measurements and analyses of the water activation experiment.
- C. Konno: to fix dpa problems in affected files and send to the IAEA for inclusion in the FENDL-3.2 library.

2.10 M. Loughlin, FENDL Meeting: ITER Perspective

The construction of ITER is proceeding rapidly. First plasma in December 2025 is on schedule. Many systems are fully designed and input from nuclear analysis will not impact the design. Exceptions are the content of the ports (heating and diagnostics systems) and the port cells. So, for nuclear analysis the next important milestone is the updating of the licensing documents (RPrS). This requires analysis based on updated and referenced data. This is FENDL. It will be used to establish the shielding, activation and radiation levels in and around ITER during operation and maintenance periods. In the latter case activation is the crucial issue.

ITER requests and would support IAEA initiatives for the provision of: activation data for all structural materials, cooling fluids and impurities found in these materials; recommendation on methods to determine neutron production from charged particle reactions on light materials (especially beryllium); specifically designed 3D computational benchmark and improved V&V of FENDL; more reliable version of NJOY or an alternative processing code; and agreement with FENDL users on setting of priorities so FENDL library can be completed.

Discussion

- ITER requests to have Ne, ^{62}Sm, ^{180m}Ta, ^{234}U, added to the transport library. Assessment of the available data leads to the following recommendation: use data from TENDL-2017; ^{234}U in TENDL-2017 below 20 MeV was adopted from ENDF/B-VIII.

- For photon-induced reactions, it is recommended to use IAEA Photonuclear Library. The ^{9}Be evaluation is coming from CNDC. There might be the need to produce ACE libraries.
- IRDFF-II data for gas production in Boron accounts for measurement at 14 MeV, which indicates significantly higher helium production for both isotopes above several MeV incident energy. It is recommended to use IRDFF-II for gas production responses in Boron and Lithium.
- Regarding the warning messages from MCNP as reported, it is assumed that they can be ignored.
- IAEA-NDS will conduct an exercise to compare capabilities of several processing codes (different levels of completeness) for production of ACE files (https://www-nds.iaea.org/index-meeting-crp/TM-Nuclear%20Data%20Processing/).
- ITER needs on uncertainty and covariance information will be detailed in a priority list.

Actions

- R. Capote: to provide links to the IAEA Photonuclear Library, to IRDFF-II library and IRDFF-II paper to ITER.
- A. Trkov: to contact L. Snoj on water activation experiments at the TRIGA reactor.
- M. Loughlin: to provide priority list of needs for uncertainty and covariance information to Andrej.

3. Discussions, Decisions and Recommendations

3.1 FENDL activation library

The previous Consultants' Meeting in 2018 recommended to introduce a TENDL-2017 based (neutron induced) activation library to substitute the FENDL3.0/A in a future release. A. Ignatyuk raised concerns about the performance of the TENDL-2017 neutron activation file due to missing adjustment to experimental data. D. Leichtle pointed out that in past years, efforts in the framework of the EURO fusion PPPT program have been conducted to improve the evaluation of important activation channels in TENDL following an updated priority list. Several V&V activities, covering integro-differential comparisons and validation benchmarking, are documented in dedicated project reports. On this basis TENDL-2017 neutron activation file has been adopted as reference library in EURO fusion PPPT neutronics superseding EAF-2007/2010.

J-C. Sublet explained that due to the new "autonorming" procedure in the TENDL-system after 2014, agreement to experimental data and specific preferential evaluations has been improved. The activation file is processed from the general-purpose file using PREPRO and NJOY. It contains sections for KERMA, dpa and gas production calculations.

R. Capote added, that generally IRDFF-II is superior to TENDL-2017, which contains data from IRDFF-1.05. The recommendation of the previous meeting, therefore, has been reconfirmed with the addition to use data from IRDFF-II, whenever available, in preference to TENDL-2017. Library and supplementary documentation will be provided to the project.

Decision

FENDL-3.2 will adopt TENDL-2017 neutron activation file as part of the activation library FENDL-3.2/A with the following recommendation:

Recommendation

Where data in the ENDF-file of IRDFF-II are available, they shall be taken in preference to TENDL-2017.

Actions

- J-C. Sublet, D. Leichtle: to provide (P)ENDF of TENDL-2017 neutron activation file to the IAEA.

- D. Leichtle: to contact U. Fischer on documentation (EU DEMO) for V&V of TENDL-2017 neutron activation file and to provide it to the IAEA.
- T. Eade: to contact Mark Gilbert for V&V on TENDL charged particle activation; provide info to A. Trkov.

3.2 Processing issues

Various issues with the processing of FENDL libraries have been repeatedly reported. Relevant information about the processing of FENDL is contained in INDC(NDS)-0611 and in collection of NJOY input files on the FENDL Library web page. A. Trkov raised concerns about the complications in updating and patching NJOY2016 in contrast to the UPD-based system of NJOY2012. NJOY2012 patches are still maintained by Skip Kahler. FENDL-3.1d has been processed with NJOY2012.50 with local updates (upnea131). As NJOY2012 is not any more available for new users, several participants suggested to move to NJOY2016 and to make use of a specific branch for the FENDL processing. The traceability of the processing is a key requirement of Quality Assurance as well as its reproducibility.

3.3 Use of application libraries

Due to partially redundant nuclear data and calculation routes for nuclear responses such as nuclear heating, damage and particle production, it has been suggested to provide specific recommendations to users. It is understood that preference should be given to evaluations from dedicated dosimetry and other application libraries. The participants concluded after some discussion with recommendations concerning a hierarchy of nuclear data for such applications.

Recommendations

For nuclear heat (prompt interactions) calculations total KERMA (MT301) from the transport library should be used. Additionally, TENDL-2017 data could be utilized by providing a respective “dosimetry” material to MCNP or by folding with a suitable incident particle flux spectrum.

For damage (DPA) calculations it is recommended to use the damage energy data (MT444) from TENDL-2017 activation file and not from the FENDL transport file.

For particle production calculations (e.g. gas production), for activation and dosimetry applications it is recommended to use IRDFF-II, when available. For the remainder, data should be taken from TENDL-2017 activation file.

3.4 Proton file for FENDL3.2

C. Konno recalled Kunieda’s presentation from the last Consultants’ Meeting 2018 which contained recommendations for the proton library of a next FENDL release. Kunieda presented improved evaluations for proton-induced reactions on $^{6/7}$Li and ^{9}Be. It is recommended to include the data in FENDL-3.2 proton induced transport library. It is also expected that other proton induced evaluations from JENDL-4.0/HE might be recommended.

Actions

- S. Nakayama: To provide $^{6/7}$Li and ^{9}Be proton transport files to the IAEA.
- S. Nakayama: to contact S. Kunieda for additional recommendations for improved p-induced files from JENDL-4.0/HE to FENDL-3.2; in this case, to provide files to A. Trkov.

3.5 FENDL-3.2 planning and beyond

R. Capote introduced the topic stating that it is planned to release FENDL-3.2 by end of 2019. It will consist of all ENDF files, whereas processed libraries will be provided in a later stage following the standard. Our effort needs to be focused on delivery of the release. The release of processed libraries is planned for summer 2020. The transport libraries for benchmarking will be made available together with the release.

A paper publication was suggested aiming to publish in NDS (special issue, appearing early 2021). This would require submitting a full document ready by summer 2020. M. Sawan explained that previously, specific papers have been published on selected topics of the FENDL activities (e.g. benchmarking). The FENDL-3.2 paper will incorporate description of library content and various benchmarking. The participants proposed responsible persons to coordinate the work and material towards the publication: R. Capote (description of library), JC Sublet/T. Eade (activation benchmarking), U. Fischer/A. Trkov (transport benchmarking). A list of all contributors to FENDL-3.2 needs to be established.

The issue was raised, that benchmarking (V&V) likely requires significant effort after the release of FENDL-3.2. Priorities of selected work required for the publication need to be defined. New evaluations in FENDL-3.2 are covered to a large extent by available benchmarking (e.g INDEN ^{56}Fe).

Touching upon the situation after the release of FENDL-3.2 and the retirement of A. Trkov, R. Capote stated that IAEA-NDS remains committed to continue the FENDL project. The continued users' feedback and request is key to steer the future development of the FENDL library.

4. List of decisions and recommendations

- FENDL-3.2 will adopt ^{56}Fe file from INDEN, version "X29r34".
- FENDL-3.2 will adopt ^{16}O-file provided by C. Konno/S. Kwon(S. Kunieda).
- FENDL-3.2 will adopt deuteron transport files from S. Nakayama, if available in due course.
- FENDL-3.2 will adopt TENDL-2017 neutron activation file as part of the activation library FENDL-3.2/A with the below recommendation:
    - Where data in the ENDF-file of IRDFF-II is available, it shall be taken in preference to TENDL-2017.
- FENDL-3.2 charged particle induced activation files will adopt TENDL-2017 (explicit channels) with the below recommendation:
    - Where data in the ENDF-file from incident charged-particle medical isotope cross section data (https://www-nds.iaea.org/medical/) is available, it shall be taken in preference to TENDL-2017.
- For specific nuclear responses, the following recommendations are provided:
    - For nuclear heat (prompt interactions) calculations total KERMA (MT301) from the transport library should be used. Additionally, TENDL-2017 data could be utilized (by providing a respective "dosimetry" material to MCNP or by folding with a suitable incident particle flux spectrum).
    - For damage (DPA) calculations it is recommended to use the damage energy data (MT444) from TENDL-2017 activation file and not from the FENDL transport file.

- For particle production calculations (e.g. gas production), for activation and dosimetry applications it is recommended to use IRDFF-II, when available. For the remainder, data should be taken from TENDL-2017 activation file.

Appendix 1

EVT1805431

Technical Meeting on the Nuclear Data for Fusion Neutronics (FENDL)

IAEA Headquarters, Vienna, Austria
2-5 September 2019
Meeting Room C0343

AGENDA

Monday, 2 September

08:00 – 09:00	**Registration** (IAEA Registration desk, Gate 1)
09:30	**Opening Session** Welcoming address – A. Koning Introduction – A. Trkov Election of Chairman and Rapporteur Adoption of Agenda Administrative matters
09:30 - 12:30	**Presentations by participants** **Presentation by Ms S. Kwon** (~ 60 min') Benchmark test for next FENDL **Presentation by Mr L. Leal** (~ 30 min') Angular data from resonance parameters, is it a viable Option? **Presentation by Mr C. Konno** (~ 60 min') Follow-up from previous FENDL meeting **Presentation by Mr A. Ignatyuk** (~ 25 min') Test of the FENDL-3.1 activation data against the revised experimental data for the charged-particle induced reactions
12:30 – 14:00	***Lunch***
14:00 – 17:30	**Presentations by participants**

Presentation by Mr S. Nakayama (~ 20-30 min')

Introduction of a computational code for deuteron-induced reactions and development plan of deuteron nuclear data files

Coffee breaks as needed

Tuesday, 3 September

09:00 - 12:30 **Presentations by participants**

Presentation by Mr M. Fabbri (~ 30 min')
A test suite for fusion library

Presentation by Mr M. Sawan, (~ 30 min')
on UW-Madison Neutronics Activities to support FENDL

Presentation by Mr D. Leichtle, (~ 30 min')
Considerations on V&V needs for FENDL data and application

Presentation by MrT. Eade, (~ 30 min') UKAEA
experiences with FENDL

12:30 – 14:00 ***Lunch***

14:00 – 17:30 **Presentations by participants**

Coffee breaks as needed

19:00 ***Dinner at Restaurant "Zum Schinakel"***

Wednesday, 4 September

09:00 - 12:30 **in-depth discussions**

12:30 – 14:00 ***Lunch***

14:00 – 17:30 **in-depth discussions**

Coffee breaks as needed

Thursday, 5 September

09:00 - 16:00 **Drafting of the summary document**

Finalisation of the Summary Report and Action List

16:00 Closing of the meeting

Coffee break(s) and lunch in between

Appendix 2

Technical Meeting on the Nuclear Data for Fusion Neutronics

2 to 5 September 2019
IAEA, Vienna

List of Participants

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Appendix 3: Links to Presentations

ID	Author	Title	Link
1	S. Kwon	Benchmark test for next FENDL	PDF
2	L. Leal	Angular Data From Resonance Parameters, is it a viable option?	PDF
3	A. Ignatyuk	Test of the FENDL-3.1 activation data against the revised experimental data for the charged-particle induced reactions	PDF
4	C. Konno	Follow-up from previous FENDL meeting	PDF
5	S. Nakayama	Introduction of a computational code for deuteron-induced reactions and development plan of deuteron nuclear data files	PDF
6	M. Sawan	UW-Madison Neutronics Activities to support FENDL	PDF
7	M. Fabbri	A test suite for fusion libraries	PDF
8	D. Leichtle	Considerations on V&V needs for FENDL data and application	PDF
9	T. Eade	UKAEA Experiences with FENDL	PDF
10	M. Loughlin	FENDL Meeting: ITER Perspective	PDF

List of actions

Note: Actions required for FENDL-3.2 assembly are highlighted.

ID	Action	When	Who	Status
A1	Compare INDEN Fe-56 file versions (r2 vs. r34)		A. Trkov	CLOSED
A2	Contact Kunieda for his evaluation ; to send new 16O-file ("new2").	Oct-19	S. Kwon/C. Konno	
A3	Produce ENDF-file from incident charged-particle medical isotope cross section data	Dec-19	A. Trkov	
A4	Assess the feasibility to merge TENDL-2017 and medical isotope cross section data in a single FENDL activation library	Dec-19	R. Capote/J-C. Sublet	
A5	Compare (d,p)-reactions in TENDL-2017 with FENDL3.0 (renormalized by A. Ignatyuk)	Dec-19	JC Sublet	
A6	Test KERMA for INDEN Fe-56	Sep-19	C. Konno	
A7	Provide modified NJOY-HEATR module to FENDL	Sep-19	C. Konno	
A8	Assess the impact of HEATR modifications from JAEA	Oct-19	A. Trkov/J-C. Sublet	
A9	Send modified 39/40-K ENDF files to A. Trkov	Oct-19	C. Konno	
A10	Assess modified files (39/40-K) to adopt them for FENDL3.2	Nov-19	A. Trkov	
A11	Provide deuteron files for 6/7-Li to FENDL	Dec-19	S. Nakayama	
A12	Provide deuteron files for 9-Be and 12-C to FENDL	Dec-19	S. Nakayama	
A13	Check status and possibility to adopt deuteron files for FENDL3.2 (by 12/2019).	Dec-19	A. Trkov	
A14	Perform FNS Cu benchmarking	Nov-19	S. Kwon	
A15	Contact M. Angelone for FNG Cu benchmarking; if not available to perform the benchmarking	Nov-19	C. Konno	
A16	Perform criticality benchmarks for Cu data (for JENDL4.0-HE)	Sep-19	A. Trkov	
A17	Repeat the calculations using the standard Cf-252 source from IRDFF-II	Nov-19	T. Bohm	
A18	Provide model and documentation of 1D-FNSF to FENDL	Dec-19	T. Bohm	
A19	Setup a repository for computational benchmark files (models, inputs, specification, etc.)	Dec-19	A. Trkov	
A20	Prepare the ITER C-lite computational benchmark input; to provide it to Andrej	Dec-19	E. Polunovskiy, M. Fabbri	
A21	Check availability of previous (simple) DONES facility model for inclusion in the computational benchmark repository.	Sep-19	D. Leichtle	
A22	Check availability of 1D-DEMO model (with breeding blanket options) - for inclusion in the computational benchmark repository.	Sep-19	D. Leichtle	
A23	Contact I. Kodeli and OECD/NEA (M. Fleming) concerning synergies with WPEC SG47	Sep-19	M. Fabbri	
A24	Outline a document on V&V procedures for FENDL	Jan-20	M. Fabbri/D. Leichtle	
A25	Provide data of measurements and analyses of the water activation experiment	Dec-19	T. Eade	
A26	Fix dpa problems in affected files and send to Andrej	Oct-19	C. Konno	
A27	Contact Mark Gilbert for V&V on TENDL charged particle activation; provide info to Andrej	Sep-19	T. Eade	
A28	Provide links to the IAEA Photonuclear Library, to IRDFF-II and to IRDFF-II paper to ITER	Sep-19	R. Capote	
A29	Contact L. Snoj on water activation experiments at the TRIGA reactor		A. Trkov	CLOSED
A30	Provide priority list of needs for uncertainty and covariance information to Andrej	TBD	M. Loughlin	

ID	Action	When	Who	Status
A31	Provide (P)ENDF of TENDL-2017 neutron activation file to Andrej	Sep-19	J-C. Sublet, D. Leichtle	
A32	Contact Ulrich on documentation (EU DEMO) for V&V of TENDL-2017 neutron activation file and provide it to Andrej	Sep-19	D. Leichtle	
A33	Provide JAEA/QST tools for ACE data interrogation to Andrej	Sep-19	C. Konno	
A34	Provide 6/7-Li and 9-Be proton transport files to Andrej	Sep-19	S. Nakayama	
A35	Contact Kunieda for additional recommendations for improved p-induced files from JENDL-4.0/HE to FENDL3.2; in this case, provide files to Andrej	Sep-19	S. Nakayama	
A36	Decide on which Cu evaluation to be adopted for FENDL3.2	Dec-19	A. Trkov	

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