Comparative survey of evaluated nuclear data libraries for fusion-relevant neutron activation spectrometry

Prasoon Raj[1,*], *Ulrich* Fischer[1], *Axel* Klix[1], and *JET* Contributors[**]

[1]Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz Platz 1, 76344, Eggenstein-Leopoldshafen, Germany

Abstract. The neutron flux-spectrum in a fusion device is frequently determined with activation foils and adjustment of a guess-spectrum in unfolding codes. Spectral-adjustment being a rather complex and uncertain procedure, we are carefully streamlining and evaluating it for upcoming experiments. Input nuclear cross-section data holds a vital position in this. This paper presents a survey of common dosimetry reactions and available data files relevant for fusion applications. While the IRDFF v1.05 library is the recommended source, many reactions of our interest are found missing in this. We investigated other standard sources: ENDF/B-VIII.0, EAF-2010, TENDL-2017, JENDL-4.0 etc. And, we analysed two experiments to ascertain the sensitivity of the spectral adjustment to the choice of nuclear data. One was performed with D-D (approx. 2.5 MeV peak) neutrons at the Joint European Torus (JET) machine and another with a white neutron field (approx. 33 MeV endpoint energy) at Nuclear Physics Institute (NPI) of Řež. Choice of cross-section source has affected the integral fluxes (<5%), reaction rates (<10%), total fluxes in some sensitive energy-regions (>20%) and individual group fluxes (<30%). Based on this experience, essential qualitative conclusions are made to improve the fusion activation-spectrometry.

1 Introduction and Objectives

1.1 Activation Foil Spectrometry in Fusion

Accurate measurement of the flux-spectrum of neutrons is an essential element of the diagnostics of a nuclear fusion device. There are only a few neutron detector-types which can be applied for this due to the need for them to sense a wide energy-spectrum, and to tolerate the harsh radiation, electromagnetic and high-temperature conditions [1]. More so difficult than the direct monitoring of the integrated flux-density is the task of spectrometry of neutrons. One tool which has been in common use for this purpose is the activation foil spectrometry using the *neutron activation systems (NAS)*. The method implements miniature samples (in the form of thin foils, wires, pellets etc.) of selected pure materials as neutron probes. Such a probe is irradiated during a plasma pulse in a location close to the plasma wall. After that, its gamma-rays emission spectrum is measured using a high-efficiency gamma spectrometer. The post-analysis of the gamma-spectrum gives rates of the reactions in the material, which in-turn can be employed to obtain the flux-densities. To obtain the energy-distribution of neutrons, multiple appropriately-chosen materials are introduced in the sample. Such a *multi-foil sample* should provide numerous reactions with varying threshold energies, dividing the range of neutron-energies into many groups. The resulting coarse flux-spectrum can be further used in extensive mathematical techniques, along with additional a-priori information about the experiment to produce a finer spectrum, in a process usually called as *spectral unfolding or adjustment*.

Typically, tokamaks and other bigger devices are equipped with automated, gas-driven tubes, known as *pneumatic transport systems (PTS)*, for transport of the samples between the irradiation ends, storage and gamma-measurement stations. The JET device in Culham (UK) [2], NPI's cyclotron-based white neutron source [3] and many planned facilities, like ITER [1] and its Test Blanket Modules (TBM) [4], the High-Flux Test Module (HFTM) of the Early Neutron Source (ENS) [5], etc. feature such integrated PTS for high-energy neutron spectrometry.

1.2 Spectral-adjustment and Nuclear Data

The two main aspects of the design of a fusion NAS include selection of materials for the probe and the integration of the intrusive PTS in compact designs of the devices. Notwithstanding another difficult part of this diagnostics, which is the post-processing of the NAS data and their use in the unfolding of the spectrum. Unfolding or adjustment requires as input total reaction rates and cross-sections. The latter is usually given as the so-called energy-wise *response functions*. A final input is the *guess-spectrum*, for which Monte-Carlo simulations are performed with descriptive modelling of the geometry and the materials at the experimental position. Simply put, an unfolding code adjusts this spectrum so that the

*Corresponding author: since Feb. 2020 at Khalifa University, Abu Dhabi, UAE, email ID: prasoon.raj@kit.edu prasoon.raj@ku.ac.ae

**See the author list of "*Overview of the JET preparation for Deuterium-Tritium Operation*" by E. Joffrin et al. to be published in Nuclear Fusion Special issue: overview and summary reports from the 27th Fusion Energy Conference (Ahmedabad, 22-27 Oct. 2018)

reaction rates calculated with this matches the ones measured. At KIT, we have been studying the sensitivity of the resulting flux-spectrum towards the choices of the input a-priori data and the boundary conditions [6]. We have utilized experimental data from JET [7], NPI [5] etc. for this purpose. Our ad-hoc scripts in Python and C++ have been used for processing gamma-spectra and making necessary corrections to reaction rate data. For unfolding, we primarily have put to use an advanced code called *MAXED* [8]. It implements the so-called *maximum entropy method* for solving the multivariate systems of equations for spectral adjustment.

Adjustment problem is inherently complex and often ill-posed. One among the most critical inputs required to obtain a physically-meaningful solution is the well-qualified nuclear cross-section data for activation reactions. This is the subject matter of this paper. We have identified a set of libraries providing the data fulfilling our needs. For two completed experiments at our disposal, we utilized these libraries to perform several unfolding exercises. Comparison of results have provided us major conclusions on the sensitivity of unfolded spectra towards available choices of nuclear data, limitations of the state of affairs of activation data and necessary improvements.

2 Survey of Evaluated Data Libraries

2.1 IRDFF Library for Fusion Needs

Common fusion NAS measures neutrons over wide energy-range, from thermal energies to 14 MeV (D-T). In many existing facilities, 2.5 MeV D-D neutrons are present. While in some accelerator-based facilities, like NPI, faster neutrons up to 35 MeV are also there. Apart from cross-sections in wide energy range, NAS also requires data for individual isotope-production routes (quite often leading to an individual metastable state) instead of the total reaction cross-sections.

For checking the availability of data, we collated different dosimetry reactions from fusion or accelerator-based facilities worldwide. There were six (n, γ) reactions for thermal neutron detection. For the range near 1 MeV to 9 MeV, 12 (n, n') reactions were kept. And for higher energies, 12 (n, p), six (n, α), eight (n, 2n), and few of each of (n, np), (n, nα) and (n, 3n) reactions were included in the list. These reactions have either been used in past, are in contemporary use, or are proposed for specific reasons for use in future experiments. In sum, we looked at a variety of pure elements (more than 25 common choices), more than 50 distinct reactions, providing half-lives from few seconds up to millions of years, and threshold-energies spread from thermal energies to 20 MeV.

The most-up-to-date and recommended cross-section library for activation experiments is the IRDFF v1.05 [9], which contains about 79 dosimetry reactions with decay data. The data are carefully and thoroughly checked for comparability with experimental data in wide energy-range, and the evaluation practices adopted therein are considered better-suited for application in high-accuracy experiments. Unfortunately, a number of fusion NAS reactions are missing from IRDFF. In the survey, we found that more than half of the listed reactions were absent. Among them are thermal neutron reactions, and a lot (>10) of both mid-range threshold reactions of (n, n') type and higher-energy (<20 MeV) threshold reactions. For example, a thermal neutron reaction ^{27}Al (n, γ) ^{28}Al, proposed for fast measurement cycles in ITER TBMs [4], is missing. Similarly, ^{77}Se (n, n') ^{77m}Se reaction for D-D neutrons and ^{93}Nb (n, nα) ^{89m}Y reaction for D-T neutrons can be cited from important cases not there in IRDFF [4]. This surely limits the capabilities of NAS in fusion, and calls for an extension of the IRDFF library.

A compromise often made for unfolding, is to apply IRDFF data for available reactions and using other standard libraries for the few missing reactions. However, using data from more than one source in a single unfolding problem can lead to uncorrelated uncertainties and thus make the process inconsistent. Given this, we have looked at other libraries which might contain more of interesting reactions. We have recognized that no evaluated nuclear data library seems to provide the cross-sections for all fusion NAS reactions and in complete energy range of interest. For some reactions in the list, all libraries miss either the cross-section for specific isotope-production cross-sections or those at requisite higher energies. By far, TENDL-2017 [10] contains the most exhaustive collection of activation reactions for fusion NAS. Close to it is the EAF-2010 [11]. A number of libraries have energy-limits below 35 MeV, e.g. ENDF/B-VIII.0 [12] is up to 20 MeV and JEFF-3.3 [13] to 30 MeV. JENDL-4.0 [14], with its high-energy (HE) extension also seems to fulfil much of our needs.

2.2 Two Analysed Experimental Cases

We analysed two different experiments to more practically highlight the issue with nuclear data availability and the sensitivity of results towards choice of cross-section sources. The experiment-1 refers to the test done with a white neutron field (approx. 33 MeV endpoint energy) at NPI using Au, Y and Co foils. Experiment-2 refers to the one performed with D-D (approx. 2.5 MeV peak) neutrons at JET, using Al, Cr and Nb foils. The reader is referred to [5, 7] for further details of these experiments and to [6] for their spectrum unfolding using two different codes. Table 1 lists all the reactions for unfolding, as produced in the two data sets.

Table 1. Dosimetry reactions in the two experimental sets, where each reaction has been numbered (RRx) for reference.

Experiment-1		Experiment-2	
RR1	^{197}Au (n, 3n) $^{195m+g}$Au	RR6	^{27}Al (n, γ) ^{28}Al
RR2	^{89}Y (n, 2n) ^{88}Y	RR7	^{52}Cr (n, p) ^{52}V
RR3	^{59}Co (n, 3n) ^{57}Co	RR8	^{93}Nb (n, 2n) ^{92m}Nb
RR4	^{59}Co (n, 2n) $^{58m+g}$Co		
RR5	^{59}Co (n, p) ^{59}Fe		

Even from the eight reactions in these experiments, three are unavailable in IRDFF. In experiment-1, we deliberately kept only IRDFF reactions except one (n, 3n) reaction. However, this was not possible for experiment-2 as it contained only four usable reactions, three of which were absent from IRDFF. So, four distinct response-functions were produced using IRDFF and other libraries,

for each of the cases as shown in Table 2. In a few cases, we had to carefully combine sources in order to have complete response-functions for a fruitful unfolding, e.g. IRDFFC (experiment-1), which also is an example of the typical compromise made for using the IRDFF data.

Table 2. List of response-functions for two experiments with the code-names and source-libraries. For response-functions with combined libraries, the reaction (RRx, ref. Table 1) and its source has been mentioned in italics, apart from the main source.

Experiment-1		**Experiment-2**	
Code	**Source**	**Code**	**Source**
IRDFFC	IRDFF v1.05 *RR1 TENDL-2017*	ENDFC	ENDF/B-VIII.0 *RR8 IRDFF v1.05*
EAF10	EAF-2010	EAF10	EAF-2010
TENDL7	TENDL-2017	TEND7	TENDL-2017
JENDL4	JENDL-4.0/HE *RR2 TENDL-2017*	JENDL4	JENDL-4.0/HE

On comparison of the cross-sections extracted from different sources in the same energy-group structures, we have found that the total cross-sections in broad regions are comparable, although up to 20-30% difference in group-wise cross-sections are quite common. In some groups, much larger differences are there which can adversely affect the unfolded spectra. We specifically found up to an order of magnitude differences between group-wise cross-sections from different sources for the thermal-neutron reactions near lower-energy ends. It is worthwhile to note that such reactions are always crucial in reactor applications. How these differences end up altering the result of multidimensional unfolding problem is important to see. In our NAS applications, we strive to attain low uncertainties (below 10%) in flux-spectra and integral responses like tritium production rate, nuclear heating etc.[15]. It becomes necessary to understand all sources of error, including the nuclear cross-section data.

3 Unfolded Spectra vis-à-vis Data Choice

The guess-spectra, what are also known as the *default* or *input-spectra*, in the two aforementioned experiments were provided by Monte-Carlo calculations previously performed at the respective facilities, i.e. NPI and JET. The measured reaction rates were obtained in analyses in [5-7], the final values of which are reported in Table 3. Here, we conducted several sets of spectral unfolding runs using MAXED for both experiments. The runs differed in the input response-functions (Table 2).

From alternative flux measurements, we know that the neutron flux in irradiation position at NPI was approx. 2×10^9 cm^{-2} s^{-1} and at JET was 9.7×10^{10} cm^{-2} s^{-1}. Here, all the NAS analyses have resulted in fluxes differing from 1 to 5% from these values, which is a promising fact showing that NAS is prolific as well as critical for high-reliability neutron flux measurements in fusion devices.

In Fig. 1 (a) and (c), the input and output spectra are compared for both experiments. For better understanding, the spectra are also presented as ratios w.r.t. input spectra in (b) and (d). As it can be seen, the unfolded spectra compare well, in general, with the input ones in both the cases (Fig. 1 (a) and (c)). The powerful computational tools behind the input guess-spectra lead to make the NAS based spectrometry a tool for verification rather than an ab-initio method for spectrum determination.

We find that few spectral regions become sensitive to large adjustments. These are the regions near 12 MeV and 20 MeV in experiment-1 and that from 5 MeV to 10 MeV in experiment-2 (Fig. 1 (b) and (d)). In former, the group-fluxes are differing by up to 25%, while in latter the differences are much higher. The total flux in this region in experiment-2 differs by as much as 17%, which can be detrimental. EAF10 makes the largest changes. The next largest difference is about 100%, between JENDL4 and TENDL7. A major reason for large adjustments in some sections and differences between response-functions therein, is the cross-section distribution. But, aspects like fine energy-bin structures also affect it. In our analyses for example, we have kept the ad-hoc energy-group structures provided by the facility-owners and not changed it as per the threshold energies of the unfolding reactions we have used. These need some detailed studies in future.

Taking the IRDFFC as base for comparison in experiment-1, TENDL7 performs closest to it. The conclusion for experiment-2 is similar, making TENDL-2017 a preferable replacement for future experiments. In general, JENDL4 and EAF10 seem to provide negligible differences from each-other, albeit EAF10 produces the larger deviations in the sensitive region in experiment-2. All the used cross-sections here have been checked for good comparison with experimentally measured data, and thus we find that TENDL-2017 amongst them suitable for putting to extensive use in future. We need to mention that the EAF-2010, also being relatively complete, and arguably better suited for activation experiments, has already been employed in previous works by us.

Table 3. Reaction rate (RR) measured for different reactions in experiments 1 (Ex-1) and 2 (Ex-2). In the last four columns, the % deviations of the reaction rates calculated using unfolded spectra (with different input response-functions as shown) from the measured rates are given for their inter-comparison.

Ex-1	**RR (s^{-1})**	**IRDFFC**	**TENDL7**	**EAF10**	**JENDL4**
RR1	6.33E+05	+ 22%	+ 14%	+ 10%	+ 10%
RR2	3.69E+06	– 1%	– 11%	– 11%	– 11%
RR3	2.74E+06	– 8%	– 11%	– 14%	– 14%
RR4	1.46E+07	– 1%	– 1%	– 1%	– 1%
RR5	1.02E+06	+ 11%	+ 12%	+ 12%	+ 11%
Ex-2	**RR (s^{-1})**	**ENDFC**	**TENDL7**	**EAF10**	**JENDL4**
RR6	5.17E+05	+ 5%	+ 4%	+ 4%	+ 4%
RR7	2.47E+05	+ 3%	+ 1%	0%	– 6%
RR8	1.63E+06	+ 2%	+ 7%	+ 9%	+ 1%

The percentage deviations of the reaction rates calculated with unfolded flux-spectra of different input response-functions, from the measured ones (RR) are shown in Table 3. The values of deviations show partially the extents of adjustments done. For experiment-1, the deviations are the largest for the reactions (RR1 and RR5) producing less activities as they are typically met with the

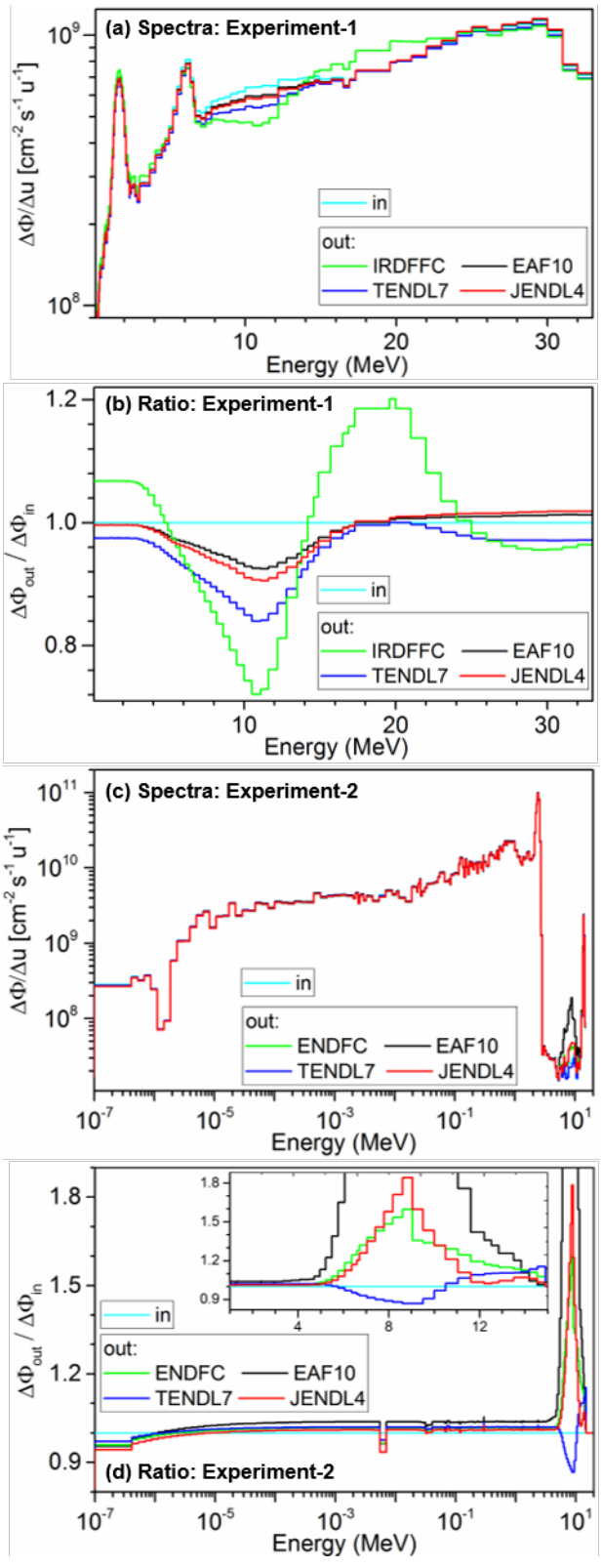

Fig. 1. Comparison of unfolded spectra for the two experiments. (a) and (b) show results from Experiment-1, while (c) and (d) from Experiment-2. (a) shows lethargy-plots for Experiment-1, where input (in) spectrum and output (out) spectra with four different response-functions are plotted versus energy. (b) shows the data of (a) in ratio form, where all group-wise fluxes have been divided by the input group-flux. Similarly, (c) shows lethargy-plots for input and output spectra from Experiment-2, and (d) the corresponding ratio plots w.r.t. energy. In the inset of (d) an expanded version of the sensitive region is shown.

largest uncertainties. If we look at the differences between response-functions with each other, the largest difference, up to 12%, is between results of IRDFFC and EAF10 in experiment-1. Similarly, a 9% difference is seen between ENDFC and JENDL4 for RR7 in experiment-2. These are marginally large differences, given that activation analyses will be frequently used to indirectly measure integral responses like tritium production rate in the reactors. These findings confide with the analyses of spectra, concluding again the need to carefully compare and select nuclear data for these experiments.

4 Conclusions

As part of the evaluation and streamlining of the fusion NAS data-processing and spectral-adjustment methodology, we have checked the level of sensitivity of output spectra to the choice of input cross-section data. Data source affects the total fluxes by up to 5%, but sensitive regions of spectra and individual group fluxes may see 30% and larger differences. As it is practically consequential, we should carefully select nuclear data for consistent and accurate unfolding. IRDFF v1.05, the recommended library for activation analyses lacks more than half of the interesting reactions in fusion NAS, and so, we propose to extend IRDFF for this application. Relatively complete sources like TENDL-2017 and EAF-2010 have been checked by us for good performance and we plan to bring them into practice for upcoming experiments. Aspects like uncertainty propagation, choice of energy-bin structure etc. are planned for future studies.

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission. The authors want to note the kind support received from L. Packer, C. R. Nobs, B. Colling and S. C. Bradnam of Culham Centre for Fusion Energy (UK), M. Majerle and M. Štefánik of NPI, and S. Simakov and A. Konobeyeev of KIT

References

1. L. Bertalot *et al*, J. Inst. **7**, C04012 (2012). doi:10.1088/1748-0221/7/04/C04012
2. R. Prokopowicz *et al*, Nucl. Instr. Meth. Phys. Res. A **637**, 119-127, (2011). doi:10.1016/j.nima.2011.01.128
3. M. Stefanik *et al*, Eur. Phys. J. Conf. **146**, (2017). doi:10.1051/epjconf/201714603011
4. A. Klix *et al*, AIP Conf. Proc. **1612** (2014) 175–178. doi:10.1063/1.4894048
5. A. Klix *et al*, Fus. Eng. Des. **146** (2019), 1258-1261. doi:10.1016/j.fusengdes.2019.02.053
6. P. Raj *et al*, Fus. Eng. Des. **146** (2019), 1272-1275. doi:10.1016/j.fusengdes.2019.02.056
7. B. Colling *et al*, Fus. Eng. Des. **136** (2018), 258-264. doi:10.1016/j.fusengdes.2018.02.005
8. M. Reginatto *et al*, Nucl. Instr. Meth. Phys. Res. A **476** (2002), 242-246. doi:10.1016/S0168-9002(01)01439-5

9. (**Webpage**) International Reactor Dosimetry and Fusion File IRDFF v.1.05, https://www-nds.iaea.org/IRDFFv105/, last accessed on May 26, 2020
10. (**Webpage**) TENDL-2017, https://tendl.web.psi.ch/tendl_2017/tendl2017.html, last accessed on May 26, 2020
11. J.-Ch. Sublet *et al*, EASY Documentation Series CCFE-R (10) 05 (2018), available online at: https://t2.lanl.gov/nis/data/jeff/EAF2010.pdf
12. D. A. Brown *et al*, Nucl. Dat. Sheets **148** (2018), 1-142. doi:10.1016/j.nds.2018.02.001
13. (**Webpage**) Joint Evaluated Fission and Fusion (JEFF) Nuclear Data Library, https://www.oecd-nea.org/dbdata/jeff/, last accessed on May 26, 2020
14. S. Kunieda *et al*, JAEA-Conf2016-004, 41-46, 2016. doi:10.11484/jaea-conf-2016-004
15. M. Angelone *et al*, Fus. Eng. Des. **136** (2018), 1386-1390. doi:10.1016/j.fusengdes.2018.05.018