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Evaluation of the spectrum unfolding methodology for neutron activation system of fusion devices

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A neutron activation system (NAS) is a highly useful and reliable tool for neutron flux and energy-spectrum measurements in fusion devices. We are evaluating a fast and efficient methodology for processing of fusion NAS data. Starting with the gamma spectra of irradiated activation materials, the method ultimately produces unfolded spectra of the incident neutrons and uncertainty estimates. Here, we test the method using data from dedicated experiments at JET and the Nuclear Physics Institute (NPI) in Řež. These measurements utilize few, from 3 to 5 reaction channels as input to the unfolding process. Two spectral adjustment code-packages have been adapted for this purpose: MAXED from UMG 3.3 and STAYSL-PNNL. While the former is frequently applied, the latter is a new addition to the case of fusion device NAS. We present the post-analyses of NAS data, spectral adjustments and some discussion on the experiences with these tools, required developments and our planned future studies.

Keywords: fusion-diagnostics, neutron-detector, activation-analysis, gamma-spectroscopy, spectrum-unfolding

1. Introduction

Neutron measurement based on activation-foils is a commonly applied diagnostic tool for fusion devices. A specific advantage of such a detector is the possibility of determining the energy-spectrum of neutrons in addition to the flux. This is done through the spectrum unfolding procedure. For the accuracy and the reliability of this method, NAS is integrated in the fusion devices and laboratories worldwide. High purity materials, chosen for their reactions having threshold energies distributed over energy-range of interest, are packaged in miniature probes. They are transported through the pneumatically-controlled pipes for irradiation and subsequent gamma-ray assaying, feeding the reactor operators and experimentalists with time-dependent neutron field information. In the KN2 laboratory of the JET device at CCFE (UK) such a system has been in place for several years [1]. Similar systems are planned for the ITER machine in Cadarache (France) [2], and the test-blanket modules (TBM) of ITER [3]. Also, this is proposed as a preferred neutron detector for envisioned material testing facilities like the early neutron source (ENS) [4].

In this paper, we examine the methodology implemented in NAS-based experiments after the stage of gamma-spectroscopy in fusion devices. It is part of the preparatory exercises for the deuterium-tritium (DT) campaign at the JET facility [5]. This campaign will provide us with a unique chance to test the activation spectrometry method in a real D-T fusion environment with wide range of energies extending to D-T neutron energies around 14 MeV. Our method starts from the measured gamma-spectrum to determine the incident neutron flux-spectrum using data-processing and spectral-adjustment tools. Here, we investigated two different unfolding codes. Our objective is to streamline the method and optimally adapt these software for our

purposes, MAXED from the UMG 3.3 package [6] and the STAYSL-PNNL suite [7]. MAXED, is a maximum entropy unfolding code, used frequently in fusion laboratories. STAYSL is a new addition to the tool-set, using an alternative, least-squares based method for spectral adjustments, accounting for uncertainties of the input data and providing group-wise uncertainties in the unfolded spectra. Here, the data-flow in the suite has been adapted for our specific problems, and results are evaluated for the needs of the field, identifying the issues and some practical suggestions. We have utilized measured activation foil data from two experiments to test the approach. In the paper, the two codes and our experiences with them, the overall method, examples of spectral adjustments, some preliminary conclusions and outlook for future developments are presented.

2. Experimental data for unfolding

Two sets of experimental data have been employed in the studies. This provided us a chance to identify practical challenges of performing spectrometry for fusion-relevant activation measurements. The outputs of an activation foil experiment are a pulse-height gamma-ray spectrum of the sample from an HPGe-type detector, and the associated irradiation, cooling and measurement times. The rates and the statistical and total uncertainties of the chosen reactions are calculated by processing these data, along with the foil masses and detector efficiencies. In Table 1, the foils, eight identified reactions, product half-lives, energy thresholds and the measured reaction rates for the two data sets are shown.

2.1 Data set-1: ENS activation foil tests at NPI Řež

The activation foil method will be implemented to measure the neutron fluence in the ENS, which is a planned facility for neutron-irradiation tests of fusion reactor materials. For the so-called high-flux test module

(HFTM) of ENS, a set of dosimetry foils have been identified and tested using a cyclotron fast neutron source at the Nuclear Physics Institute (NPI) Řež [8], where 37 MeV proton beam impinging on a heavy water (D₂O) target produces neutrons up to energy of 35 MeV. At NPI, several material probes were irradiated, with Au, Y and Co among them [9]. The facility operated over a 9.5 hour long constant-flux period with an average beam-current of 10.9 μ A and providing a neutron flux of approx. $2.3 \times 10^9 \text{ cm}^{-2} \text{ s}^{-1}$. For post-analyses, Monte-Carlo simulations for neutron-spectra were available for these tests [8]. The gamma spectrum measurements were performed three months after the irradiation. The utilization of long-lived reaction products are necessary for ENS as the probes will be extracted after cooling times ranging from weeks to months. We have selected a set of five reactions from these measurements for use in the spectral unfolding procedure (see Table 1).

2.2 Data set-2: TBM activation foil tests at JET

One of the missions of the recent campaigns of the JET device is to perform representative tests of the nuclear detectors proposed for the European TBMs of ITER. Under the umbrella of the TBMD sub-project of the EUROfusion work-package JET3 [5], this task involves, among others, the experiments for qualification of the TBM-NAS. In the deuterium-deuterium (D-D) runs concluded in 2016, a foil package containing Al, Cr and Nb was irradiated in the KN2 upper port (KN2-3U) of JET. The plasma was on for a duration of 3 seconds, with an estimated neutron flux of $9.7 \times 10^{10} \text{ cm}^{-2} \text{ s}^{-1}$. A set of three reactions were selected from the data obtained in this measurement, as shown in Table 1. In this case, a gamma spectrum from the complete package was measured in the list mode, which was read and evaluated using a Python-based toolbox developed at CCFE [10]. The reaction products here, are short-lived, which are crucial for TBM [3] as short measurement cycles are better-suited for foil irradiation with short plasma shots in tokamaks.

3. Spectral adjustment methodology

As an ultimate outcome of the activation foil spectrometry, we want group-wise neutron fluxes in the measurement position, in a fine energy-group structure, for which multiple mathematical techniques are available [11]. Additional a-priori information should be supplied to obtain physically meaningful results in an unfolding process, which is often considered an ill-posed problem.

In practical cases, the output spectrum is extracted by “adjusting” a default spectrum, which is guessed using an analytical or a computational calculation, such as a Monte-Carlo particle transport simulations. Normalized default spectra, also known as input spectra, are shown in Fig. 1. For the NPI Řež facility, an ad-hoc 124 energy group structure ending at 35 MeV has been used in the input spectra, whereas the standard Vitamin-J 175 energy groups are used for data set-2. We follow these respective group-structures for this paper.

With the reaction rates and input spectrum, so-called response functions are required, which are related to the

group-wise cross-sections of the reactions in the data set. We utilize the NJOY-2016 [12] evaluated nuclear data processing code for preparation of group-weighted cross-sections tables. For response function to be used in MAXED, the cross-section values are multiplied with the number of target nuclides. In STAYSL PNNL, however, the normalization with respect to the number of target nuclides has to be done in the reaction rates.

Table 1. Sets of activation foil data: foil material (Mat), mass (m) in g, reaction, product half-life ($T_{1/2}$) in s, threshold energy (E_{th}) in MeV and the measured reaction rate (RR) in s^{-1} .

Mat	m	Reaction	$T_{1/2}$	E_{th}	RR
Data set-1: ENS foils with p-D₂O 35 MeV neutrons (NPI Řež)					
AU	0.30	$^{197}\text{Au} (n, 3n) ^{195m+g}\text{Au}$	1.6×10^7	14.8	6.3×10^5
Y	0.70	$^{89}\text{Y} (n, 2n) ^{88}\text{Y}$	9.2×10^6	11.6	3.7×10^6
CO	2.79	$^{59}\text{Co} (n, 3n) ^{57}\text{Co}$	2.4×10^7	19.4	2.7×10^6
		$^{59}\text{Co} (n, 2n) ^{58m+g}\text{Co}$	6.1×10^6	10.6	1.5×10^7
		$^{59}\text{Co} (n, p) ^{59}\text{Fe}$	3.8×10^6	0.8	1.0×10^6
Data set-2: TBM foils with D-D 2.5 MeV neutrons (KN2-JET)					
AL	0.07	$^{27}\text{Al} (n, \gamma) ^{28}\text{Al}$	1.3×10^2	0.0	5.2×10^5
CR	2.12	$^{52}\text{Cr} (n, p) ^{52}\text{V}$	2.2×10^2	3.3	2.5×10^5
NB	4.47	$^{93}\text{Nb} (n, 2n) ^{92m}\text{Nb}$	8.8×10^5	8.9	1.6×10^6

In the pre-analyses, we examined several sources of cross-section data for our purpose. The IRDFF [13] library is the recognized and recommended one for activation foil spectrometry, but it contains only a limited number of reactions. The STAYSL PNNL suite comes with the IRDFF data and certain features of the suite are hard-coded w.r.t. their list of reactions. For the reactions used in this work, this source was insufficient and numerous other trusted evaluated data libraries were checked. The differences in the output spectra were not drastic on changing the source of data, but about 10% changes could be seen which was critical for us. A major issue affecting our choice was the absence of covariance data for reactions and energy-ranges of interest. Covariance matrices are necessary for least-squares fitting. For consistency of results, we chose EAF-2010 [14] as the source of cross-sections and covariance for unfolding exercises shown here. MAXED-style response functions for the reactions are shown in Fig. 2.

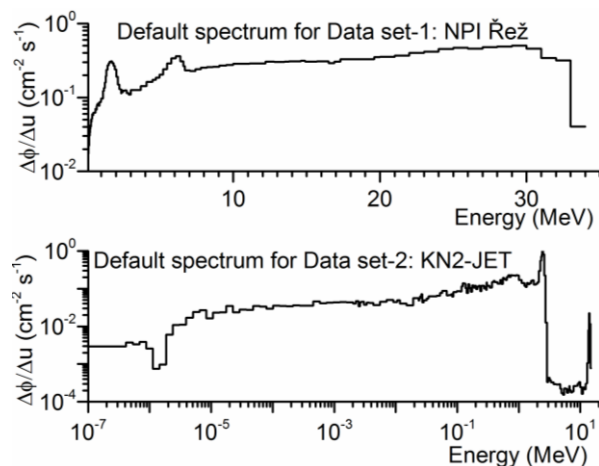


Fig. 1. Normalized lethargy plots showing the default spectra.

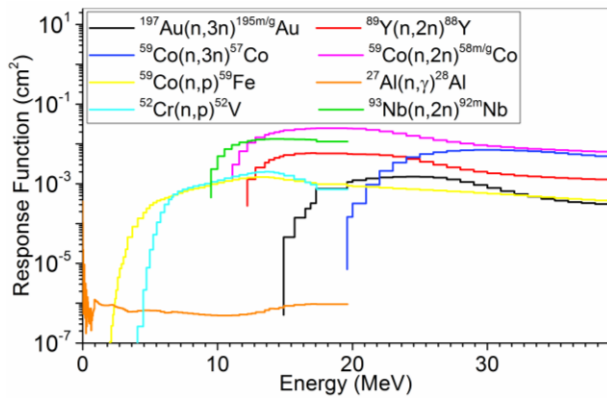


Fig. 2. MAXED-format response functions for the reactions.

To reach an optimum level of accuracy in the result, it is crucial to apply several corrections to the reaction rates and response functions. This includes factors for self-shielding of neutrons and gamma self-attenuation in the probe and the detector geometry, change in the parent nuclide density due to burnup over longer irradiation periods, decays during reactor off-times, etc.

3.1 MAXED from UMG 3.3

The maximum entropy approach has been in use in the spectral adjustment codes for many years. MAXED, now a part of the UMG 3.3 code package from NEA data bank, is a prime example of an unfolding software based on this method [6]. It has been successfully validated for fusion applications, and it is a standard tool for neutron spectrometry in most of the fusion facilities.

The a-priori information and input reaction rate data is provided for a MAXED run through four input files in text format. The control file is the one providing important values (for example, the required χ^2 and scaling and temperature reduction factors) for the algorithm and addresses for the other files. The reaction rate (in counts per second), statistical uncertainty (absolute and percentage) and uncertainty from other sources, for all reactions of the data set are given in the second file. Each reaction is identified by a unique ID, matched with the ID used in the response function file, the third file. In this file, the energy-grid-boundaries are given, along with the group-wise response function for every reaction. Finally, in the default spectrum file, the energy-grid boundaries, group-wise flux data and their respective uncertainties are supplied.

3.2 STAYSL-PNNL suite

The STAYSL code [15], employing a least-squares method for unfolding, underlies the STAYSL-PNNL suite. Along with a simple-to-use executable for the code, this package has computational tools and scripts for preparation of data to be used in the final unfolding. The reaction rate should be in units of product atoms per second per target atom. Default cross-section and covariance files containing tens of reactions from the IRDFF-V1.05 [13] data library are provided for the ease of users. For the reactions not included, this data has to be generated and added to the files using NJOY.

For a generic case, a STAYSL-PNNL run requires input and a-priori information through the case input file, cross-section file and covariance matrix file. The case file contains several flags and values to define the problem, gives the input data and mention the required outputs. Among other things, this takes reaction rate and uncertainty for each channel, energy-grid boundaries, group-wise fluxes and uncertainties for the default spectrum, and covariance matrices of flux-spectrum, input activities and cross-reaction covariance.

4. Results and discussion

In Fig. 3, the adjusted spectra for the two cases are shown. In each case, the MAXED-based and the STAYSL-PNNL (SPNNL)-based solutions are presented as lethargy plots. On the right Y-axes, the percentage difference of output group-flux ($\Delta\phi_{out}$) from the input group-flux ($\Delta\phi_{in}$) is given.

The formatting of input files is strict in both of these codes. The format of float values should also be handled with care. In many cases, the code runs successfully taking a wrong input number, especially with its exponential part, and so, a careful survey of the output file is also necessary before going to the produced spectrum. We used C++ scripts to prepare the input files on the basis of the sample cases.

The total neutron flux calculated through these codes are compared with the ones estimated. The original estimation in data set-1 was done using accelerator beam currents, and in set-2 using KN2 neutron monitor of JET. MAXED result is 7% lower in data set-1 and around 28% higher in data set-2. In energy bins groups around 10 MeV in data set-2, larger adjustments are done by MAXED. The exact reason for this is unclear and requires further scrutiny.

The SPNNL produced total fluxes differing by less than 1% from the original estimations in both the cases. It is pointed out that the tools used to guess the spectrum are rather powerful nowadays. This means that, in essence, a NAS-based spectrometer is needed to improve, and in many situations only verify, this calculated spectrum. The outcome of SPNNL is found to depend strongly upon the input uncertainties and covariance data. The covariance matrices for input spectra are required but unavailable in both the experiments, which affects the results adversely. The group-wise relative uncertainty in data set-1 is 0.86% to 1.03%. Likewise, it is 1.3% to 1.4% in data set-2. Small values of the errors reflect the small uncertainties in input reaction rates and missing covariance matrices. The code provides models to calculate the covariance for different input parameters. This is an effective tool as it can alter the output spectrum by big factors. However, a consistent way to use the inbuilt functions is lacking for our case, and is a topic for future studies.

5. Conclusions

In this paper, we have shown the testing of our methodology for spectrum unfolding starting from the activation foil data from fusion devices, implementing

the MAXED and STAYSL PNNL codes. The STAYSL PNNL has been implemented the first time for our fusion-based applications and it is found to be a promising alternative for regular use. The results of both codes agree with the estimated outcomes for the two

experimental data-sets applied for testing. Subjects for further studies are- obtaining good quality cross-section and covariance data, reliable uncertainty estimation in input spectra and looking into efficient methods of using covariance calculation models in STAYSL PNNL code.

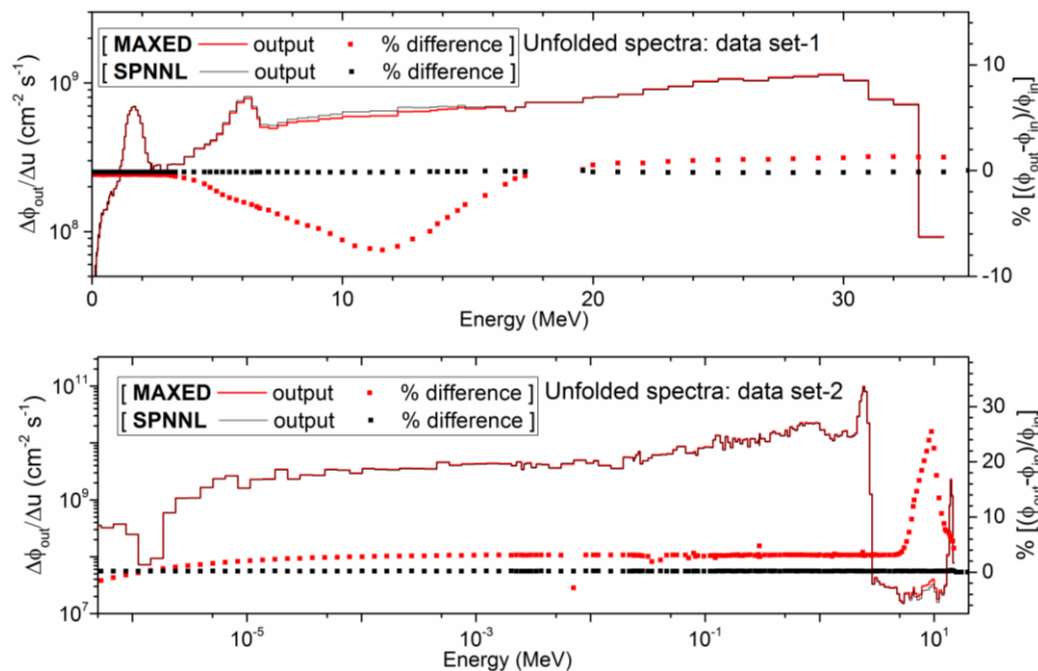


Fig. 3. Resulting neutron spectra lethargy-plots ($\Delta\phi/\Delta u$) after unfolding in MAXED (red) and SPNNL (black) for the two data-sets.

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