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Recent Progress in Neutron-, Proton- and Deuteron-induced Reaction Nuclear Data for EAF-2010 and the European Activation System

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The European Activation System (EASY) has been continuously developed and improved for more than 20 years. Its primary purpose is to carry out neutron- proton- and deuteron-induced activation calculations in support of nuclear technology, particularly for nuclear material selection, design and optimization. It comprises the EAF nuclear data libraries and the FISPACT inventory code. For fusion applications, materials used for the construction of ITER, particularly plasma facing components, will be submitted to intense neutron irradiation. These materials may be evaluated using EASY for their nuclide inventory, He gas production and decay heat production over time, for example. EASY includes data to 60 MeV, making it also relevant for IFMIF analysis, and now covers 66,256 reactions. Such large libraries require an extensive validation process, which includes the statistical analysis of cross sections (SACS) and comparisons with differential and integral data. The suite of these methods has now been extended to evaluate the next library release, EAF-2010. Furthermore, significant attention has been focused on improving the uncertainty file, a unique feature of EAF libraries. In this work we discuss recent data improvements to be included in EAF-2010 and extensions to the treatment of uncertainties both in EAF and within EASY.

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I. INTRODUCTION

High quality activation data and associated inventory codes are of fundamental importance in the development of new nuclear technology. This is particularly true for the technologies that are necessary to develop fusion power, which is a process that releases energy by recreating the physical conditions that power the sun by sustaining a high-temperature plasma that acts as an intense, high-energy neutron source. In the steps towards an operational fusion power plant the behaviour of new materials and components need to be simulated in these intense neutron fields so that one may predict the levels of activation necessary, for example, to calculate dose budgets for operations and maintenance, to predict waste inventories for decommissioning strategies, and to estimate effects such as material swelling and embrittlement. Such simulations are required to design, optimise and ultimately select promising candidate materials for components which require further qualification and testing in high neutron flux irradiation fields, such as IFMIF and component testing facilities (CTF).

The European Activation File (EAF), which is part of the European Activation System (EASY), has been developed over more than 20 years and includes data for neutron-induced reactions up to 60 MeV. These data meet some of the needs to simulate nuclear interactions for fusion devices such as ITER and covers the neutron spectrum energy range required for the materials testing facility IFMIF. EASY also includes data and tools to calculate activation due to deuterons and protons.

In addition to cross section data, activation calculations need an inventory code and evaluated decay data. EASY uses the FISPACT inventory code for calculation [1]. The various parts of EASY-2010, which is expected to be released in mid-2010, are described below.

II. EASY-2010

Several components of the EASY-2010 package have been released, including the EAF-2010 point- and group-wise neutron cross section files [2], the decay data files [3] and the biological hazard data files [4]. The full

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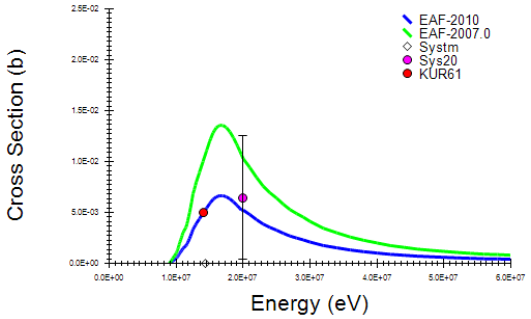

Fig. 1. (Color online) Data from EAF-2007 and EAF-2010 (Final) for ^{7}Li(n,d)^{6}He.

release will also include the FISPACT inventory code executable for Windows and UNIX platforms and the deuteron and proton libraries. A future version of EASY is also planned to include a new graphical user interface. All parts of EAF-2010 have been constructed using the SAFEPAQ-II application [5].

1. FISPACT inventory code and future developments

The FISPACT code has been updated from the previous version to handle the new, extended EAF-2010 nuclear data files. It is able to make calculations for activation by neutrons, deuterons and protons. An important feature for the three incoming particles is the listing of the pathways for the production of the dominant nuclides.

Major work is underway for a future, successor code to FISPACT to extend the functionality and range of applications. It is planned that it will include the treatment of α-, γ-, n-, p- and d-induced transmutation, generation of emitted particle spectra, physics treatment for temperature dependent cross sections, self-shielding corrections and inclusion of new multi-group structures.

2. EAF-2010 neutron-induced data

EAF-2010 contains a point-wise neutron-induced cross section library with data for 66,256 cross sections for 816 targets. 691 reactions and two additional nuclides have been added to this library in comparison to the previous release, EAF-2007. A set of eleven multi-group libraries are generated from this library with various spectra weightings, these are used as input by FISPACT. Feedback from the activation handbook produced using EAF-2007 [6] was used to improve the data in EAF-2010.

An example of improved data in EAF-2010 is shown in Fig. 1 for ^{7}Li(n,d)^{6}He. The new data are in better agreement with the 20 MeV systematic and the Mikhaylina *et al.*, 1961 experimental point at 14.1 MeV, taken from the EXFOR database [7].

3. EAF-2010 uncertainty file

The uncertainty file is used by FISPACT so that uncertainty estimates can be made for activation calculations. It contains up to four values covering different energy regions for each reaction. The error factor, $f = 1 + \Delta$, where Δ is the relative error of the cross section stored in the library. The best estimate of the cross section is $\frac{\sigma}{f} \leq \sigma \leq \sigma f$. Several improvements to the uncertainty file have been made, including the reassessment of some error factors. New consistent rules have been introduced for the determination of uncertainties for threshold reactions with experimental information. They are sensitive to the position of the experimental data on the excitation function and thus give a better representation of the adopted uncertainty with respect to the energy dependence. A new treatment has been also introduced for data with split cross-section to isomeric states, if only one of the uncertainties is known experimentally. New error factors have been introduced for non-threshold reactions which have no supporting experimental data (score = 0). These factors have been derived from cross section systematics. Some revisions have been made for non-threshold (score > 0) reactions. A new semi-quantitative approach has been used for error factors in the 1/v and <100 keV regions, which are based on error propagation of cross sections at thermal neutron energies and resonance integrals with corresponding C/E values.

4. EAF-2010 deuteron and proton-induced data

Deuteron- and proton-induced libraries were originally distributed as part of EAF-2005.1. Improvements to the data were made and incorporated into EAF-2007 and EAF-2010 uses this data. Further improvements to these libraries are planned to be advanced in tandem with new activation code developments. The current deuteron library contains 66,864 cross sections for 810 targets and the proton-induced cross section data contains 67,925 cross sections on 803 targets (based completely on TALYS calculations using global parameters [8]). Multi-group data are available in a 211-group structure (modified VITAMIN-J) extending up to 55 MeV.

5. EAF-2010 decay data

EAF-2010 contains decay data for 2,233 nuclides. The primary source is the JEFF-3.1.1 library [9]. Although the JEFF-3.1.1 library is very extensive, many of its data lack γ emission data. Such data are important for activation calculations (γ dose rate) and so the JEF-2.2 library [10], used in previous EAF versions, was also used for EAF-2010. Recent UK evaluations [11,12], not available for JEFF-3.1.1, have also been used for EAF-2010 where possible. Compared to EAF-2007 an additional 43 nuclides have been added from UKPADD sources and more than 1600 nuclides have been updated from the JEFF-3.1.1 source.

6. SAFEPAQ-II

SAFEPAQ-II [5] is the software application used to organise, view, alter, process, analyse and modify activation data. It has been used to test and validate all EAF library components. The tool stores data in relational databases and provides an interactive method to view all the data sources and experimental data (differential

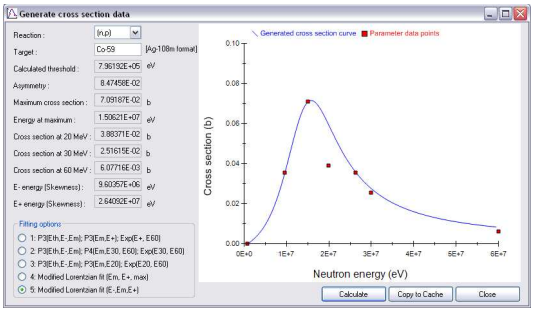

Fig. 2. (Color online) Generate cross section data tool for threshold reaction types, implemented in SAFEPAQ.

and integral). Various modification types can be implemented to improve the data. Validation of EAF neutron libraries compared to integral data, and the statistical analysis of cross section (SACS) analysis, described below, are carried out with SAFEPAQ-II.

A new feature for analysis developed during the production of EAF-2010 is the ability to produce cross section curves for threshold reactions based on the fits in the Analysis tool. This feature may be used by the evaluator to generate data, for example, if there are no other sources available. A screen shot of the tool is shown in Fig. 2.

III. VALIDATION OF EASY

During library construction, comparison with the differential data in EXFOR and with various systematics is done to ensure the library data are as correct as possible. An important additional step in validation is the comparison with integral data. This is underway at present for EASY-2010; details of the previous exercise on EASY-2007 [13] are reported here for illustration.

The methodology for this comparison in SAFEPAQ-II is different from that used in other studies. Usually the activity of a measured nuclide (E) is compared with a calculated value (C) using the library data. Thus the C/E values are quoted for various radionuclides. In SAFEPAQ-II the reaction producing the nuclide is identified and its average cross section in the neutron spectrum is used as E. Similarly the library data are averaged in the neutron spectrum to form C. Thus C/E refers to a ratio of average cross sections for the reaction forming the spectrum for the radionuclide of interest.

Using this method, effective cross sections for a wide range of reactions measured from several sources were entered into SAFEPAQ-II. A plot of the C/E values for the ^{54}Fe(n,p)^{54}Mn reaction is shown in Fig. 3. The experimental uncertainty of the measurement is shown by the error bar and the EAF library uncertainty by the error band. In this case all the error bars overlap the uncertainty band, except two, indicating reasonable agreement of the library data with the measurements.

It is always necessary to consider the differential data for the reaction in addition to the integral data; these are shown in Fig. 4. Note that experimental data extend up

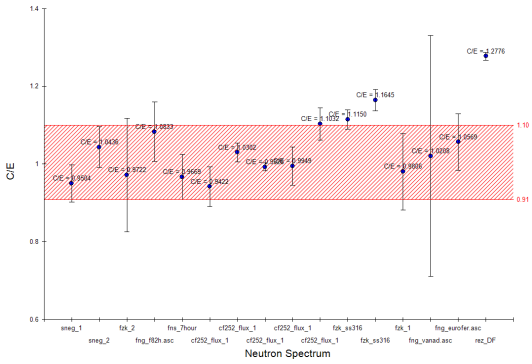

Fig. 3. (Color online) C/E data for ^{54}Fe(n,p)^{54}Mn measured in various neutron spectra. The band indicates the uncertainty in the library.

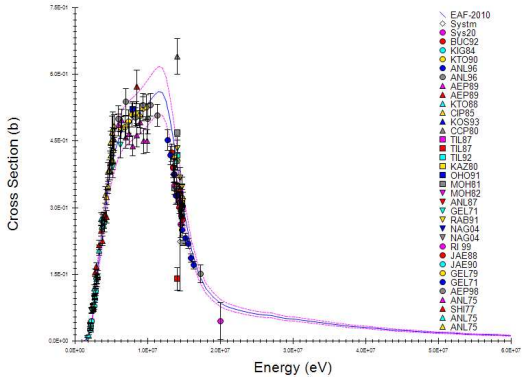

Fig. 4. (Color online) Cross section data for ^{54}Fe(n,p)^{54}Mn in the EAF-2010 library, the dotted line indicates the library uncertainty. The points represent measurements from EXFOR.

to about 20 MeV. Good agreement of the library data with differential and integral measurements lead to this reaction being described as 'validated', but it should be noted that there are no measurements for energies above 20 MeV so the reaction has not in fact been tested for these energies.

For the EASY-2007 validation report a total of 470 reactions were considered, of these 217 were classed as validated. A further 43 reactions which were split into ground and isomeric state showed good agreement for the sum, although the details of the splitting could not be tested. The remaining reactions either showed discrepancy of one type of data and the library or one type of data was missing. These reactions need to be improved in the EAF library or additional measurements are required.

IV. STATISTICAL ANALYSIS OF CROSS SECTIONS (SACS)

From the discussion above on library validation it can be seen that only a small fraction of the reactions in an activation library can be compared to differential or integral measurements. For EASY-2010 validation, which is underway, there are 1,728 reactions with differential

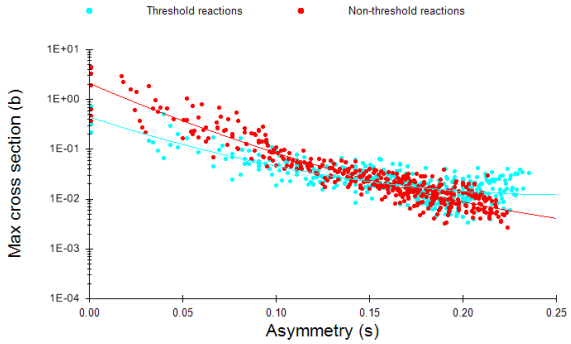

Fig. 5. (Color online) $\sigma_{\max}(s)$ for all (n,p) reactions in EAF-2010. Threshold and non-threshold reactions are distinguished. Reactions with targets A <20 are excluded.

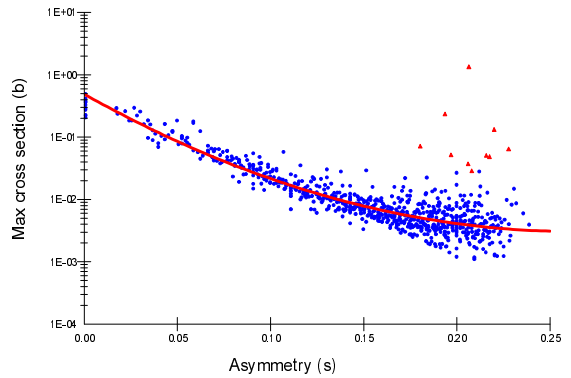

Fig. 6. (Color online) $\sigma_{\max}(s)$ for all (n,α) reactions in EAF-2005. Reactions with targets $A < 20$ are excluded.

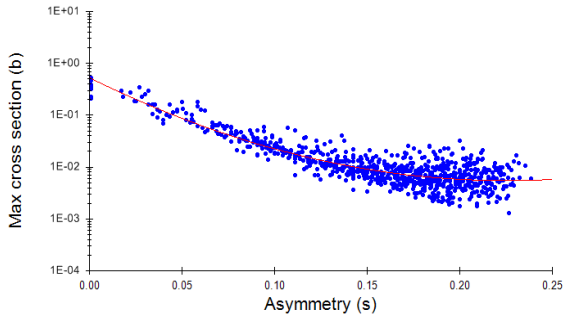

Fig. 7. (Color online) $\sigma_{\max}(s)$ for all (n,α) reactions in EAF-2010. Reactions with targets $A < 20$ are excluded.

or integral data, so some other methods are needed to test the majority of reactions. The method of Statistical analysis of cross sections (SACS) has been developed [14]. This is based on the observation that experimental data for a reaction type at a particular energy have a very good correlation with quantities like mass (A) or asymmetry parameter ($s = (N - Z)/A$). This has been used previously in the derivation of systematics. Similar effects have been seen for the maximum cross section ($\sigma_{\max}$). In SACS $\sigma_{\max}$, the energy of the maximum ($E_{\max}$) and the width at half maximum ($\Delta_{1/2}$) can be plotted as functions of A, Z or s for all reactions of a particular type in the library. An example for (n,p) data in EAF-2010 is shown in Fig. 5.

Figure 5 shows a trend line for threshold and non-threshold reactions. It can be seen that there is a well defined correlation for both data sets.

Similar curves were plotted for reactions in EAF-2005 and some points were very discrepant from the trend. These were investigated and in many cases errors in the library data were identified. An example is shown in Fig. 6 for (n,α) reactions, the very discrepant reactions around $s = 0.2$ are shown with a red triangle symbol. The improvement of the (n,α) data in EAF-2010 can be seen by comparing Figs. 6 and 7.

V. CONCLUSIONS

The various parts of EASY-2010, such as the EAF data, are described. EAF-2010 contains neutron-, deuteron- and proton-induced cross section data and some comparisons of library data with EXFOR are given. For the neutron-induced library comparison with integral data allows a minority of the reactions to be validated. All reactions can be tested by the SACS method and examples are shown.

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