

EASY-2007: a new generation of activation modelling including neutron-, proton- and deuteron-induced reactions

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Abstract. The European Activation System (EASY) has been developed for activation calculations. It comprises the EAF nuclear data libraries and the FISPACT inventory code. A new version (EASY-2007) has been released recently that represents a significant extension of previous versions. It contains neutron-induced, deuteron-induced and proton-induced data that extend up to 60 MeV. The motivation for the inclusion of charged particle induced reaction data is that such data are required for activation calculations on IFMIF, a materials testing facility. The number of reactions covered by EAF-2007 is about 200,000 which is a huge increase over EAF-2003 which contained neutron-induced data for about 12,500 reactions. Such large libraries require new methods of testing and the principles of Statistical analysis of cross sections (SACS) are outlined. This enables various quantities such as maximum cross section to be plotted as a function of asymmetry parameter for each reaction type. Such plots show well defined trends and inconsistent data for a particular reaction can readily be identified.

1 Introduction

Activation data are of fundamental importance for fusion technology. For many years in Europe there has been work on producing the European Activation File (EAF) which in version EAF-2003 [1] covered neutron-induced reactions up to an energy of 20 MeV. Such a file meets the needs of fusion devices such as ITER [2]. However, the power plants that follow ITER will subject materials to much larger neutron fluences and consequently these materials need to be tested and qualified following such irradiation. The materials test facility IFMIF [3] is planned to operate in parallel with ITER to provide this information.

IFMIF will use beams of 40 MeV deuterons striking a flowing lithium target to generate intense neutron fields. Although the neutron spectrum covers the fusion relevant energies below 14 MeV, there will be a high-energy tail extending up to about 55 MeV. In order to enable neutron activation calculations for IFMIF, cross section data in EAF-2005 [4] extended to 60 MeV. Activation due to deuterons will occur in the IFMIF accelerators and so deuteron-induced cross section data are also required. The testing phase of IFMIF may use H_2^+ beams instead of D^+ , which means that proton-induced data are needed. The newly released EAF-2007 contains cross section data for reactions induced by all three particles.

In addition to cross section data, activation calculations need an inventory code and decay data. The European Activation System (EASY) uses the FISPACT code for calculation. The various parts of EASY-2007 are described below.

2 EASY-2007

EASY-2007 [5] consists of the FISPACT-2007 [6] inventory code, the EAF-2007 neutron library [7], deuteron and proton

libraries [8], decay data [9] and biological hazard data [10]. All parts of EAF are constructed with the SAFEPAQ-II application [11].

2.1 FISPACT-2007

The FISPACT-2007 code 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.

2.2 EAF-2007 neutron-induced data

EAF-2007 contains a point-wise neutron-induced cross section library with data for 65,565 cross sections on 816 targets. 41 additional targets compared to EAF-2005.1 have been added, so that all nuclides with half-life >6 hours are included as targets. A set of eleven multi-group libraries are generated from this, these are used as input by FISPACT. An uncertainty file gives up to four values for each reaction. An example of improved data in EAF-2007 is shown in figure 1 for $^{58}\text{Ni}(n,t)^{56}\text{Co}$. The new data agree well with the recent measurements from Geel (GE06) stored in EXFOR.

2.3 EAF-2007 deuteron-induced data

A preliminary deuteron-induced library was distributed as part of EAF-2005.1. EAF-2007 contains an improved one with 66,864 cross sections for 810 targets. Multi-group data are available in a 211-group structure (modified VITAMIN-J) extending up to 55 MeV. Improvements over the previous version include data for low mass targets and renormalisation to experimental data. Most of the data are from model calculations using TALYS [12]; however the Japanese ACSELAM library [13] was also used for some reactions.

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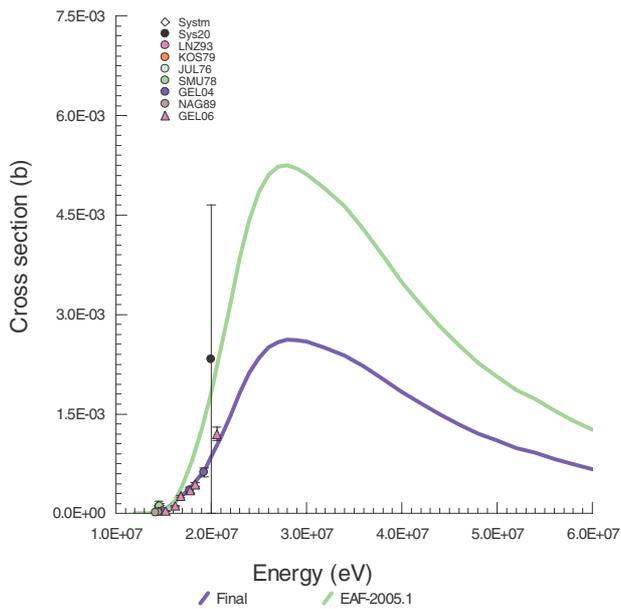


Fig. 1. Data from EAF-2005.1 and EAF-2007 (Final) for $^{58}\text{Ni}(n,t)^{56}\text{Co}$.

Figure 2 shows that EAF-2007 is in good agreement with the recent EXFOR data (NRS83), but also how large the variation between data sources can be. There is no uncertainty file for deuteron data in EAF-2007.

2.4 EAF-2007 proton-induced data

EAF-2007 contains for the first time proton-induced cross section data. The 67,925 cross sections on 803 targets are based completely on TALYS calculations using global parameters. Although experimental data are available from EXFOR no

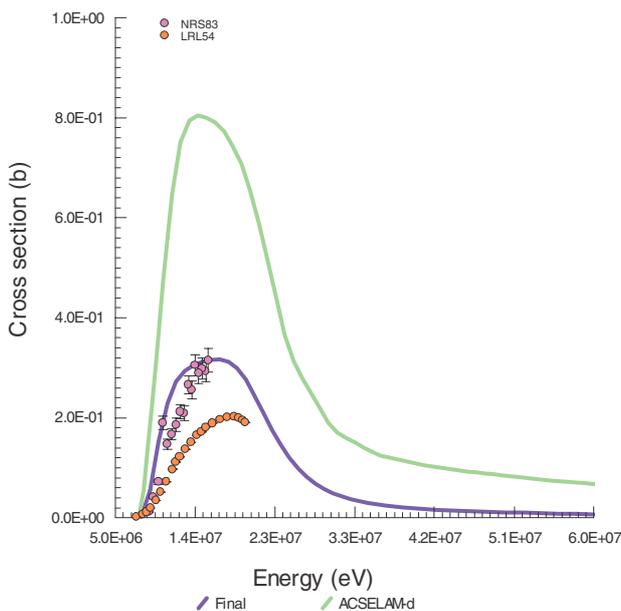


Fig. 2. Data from EAF-2007 (Final) and ACSELAM for $^{56}\text{Fe}(d,2n)^{56}\text{Co}$.

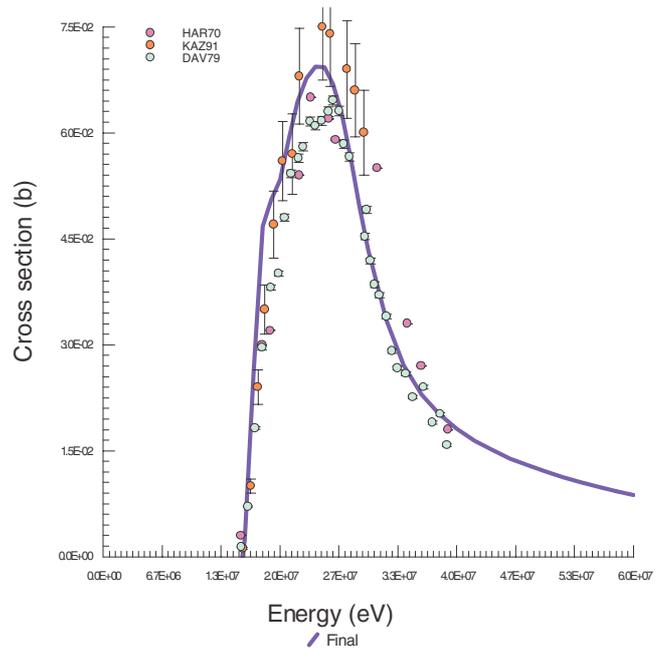


Fig. 3. Data from EAF-2007 (Final) for $^{56}\text{Fe}(p,2n)^{55}\text{Co}$.

renormalisations have been carried out. Data for H and He targets are missing, as are uncertainty data.

As with the deuteron data, multi-group data are available in 211 groups. Figure 3 shows a reaction where there is reasonable agreement with experimental data, while figure 4 shows a case with very discrepant EXFOR data.

2.5 EAF-2007 decay data

EAF-2007 contains decay data for 2,231 nuclides. The primary source is the JEFF-3.1 library [14]. Although the JEFF-3.1 library is very comprehensive, many of its data lack γ

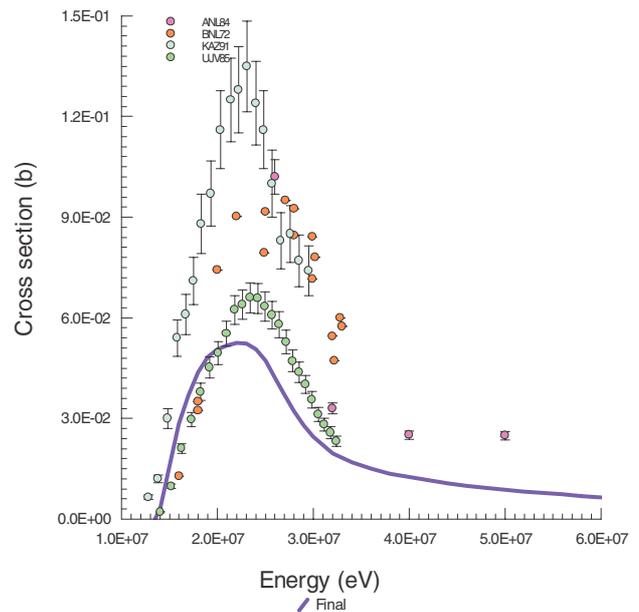


Fig. 4. Data from EAF-2007 (Final) for $^{63}\text{Cu}(p,2n)^{62}\text{Zn}$.

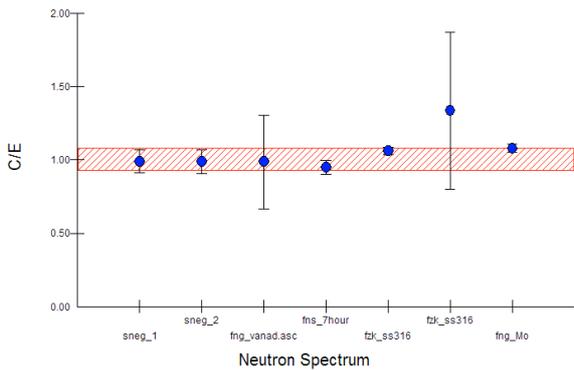


Fig. 5. C/E data for $^{100}\text{Mo}(n,2n)^{99}\text{Mo}$ measured in various neutron spectra. The band indicates the uncertainty in the EAF-2007 library.

emission data. Such data are important for activation calculations (γ dose rate) and so the JEF-2.2 library [15], used in previous EAF versions, was also used for EAF-2007. Recent UK evaluations [16], not available for JEFF-3.1, have also been used for EAF-2007 where possible. Compared to EAF-2005 an additional 40 nuclides (mostly short-lived isomers) have been added, while one (^{212}Po) has been removed.

2.6 SAFEPQA-II

SAFEPQA-II [11] is the software application used to construct all the EAF libraries. It stores data in relational databases and provides an interactive method to view all the data sources and experimental data (differential and integral). Various modifications can be defined to improve the data. Considerable extension was necessary so that deuteron- and proton-induced reactions could be treated. Validation of EAF neutron libraries compared to integral data, and the SACS analysis, described below, are carried out with SAFEPQA-II.

3 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 extremely important additional step in validation is the comparison with integral data. This is underway at present for EASY-2007; details of the previous exercise on EASY-2005 [17] are reported here for illustration.

The methodology for this comparison in SAFEPQA-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 SAFEPQA-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 in the spectrum forming the radionuclide of interest.

Using this method effective cross sections for a wide range of reactions measured as part of the EFDA Fusion Technology programme, as well as for data from the literature, were

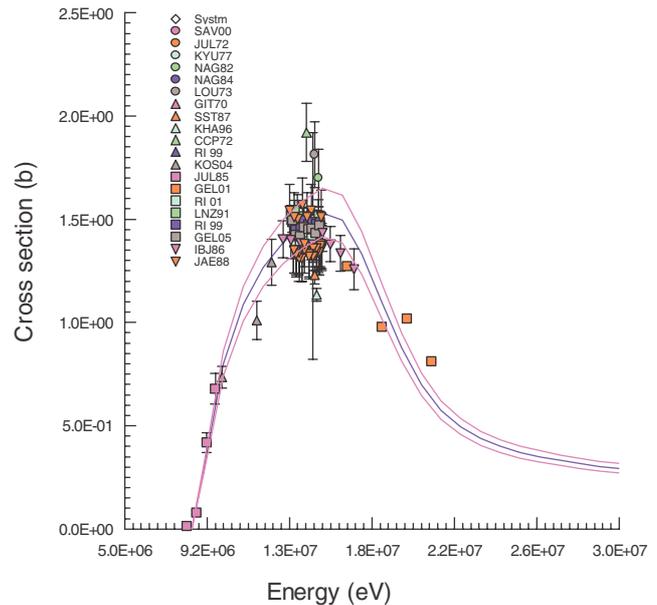


Fig. 6. Cross section data for $^{100}\text{Mo}(n,2n)^{99}\text{Mo}$ in the EAF-2007 library, the dotted line indicates the library uncertainty. The points represent measurements from EXFOR.

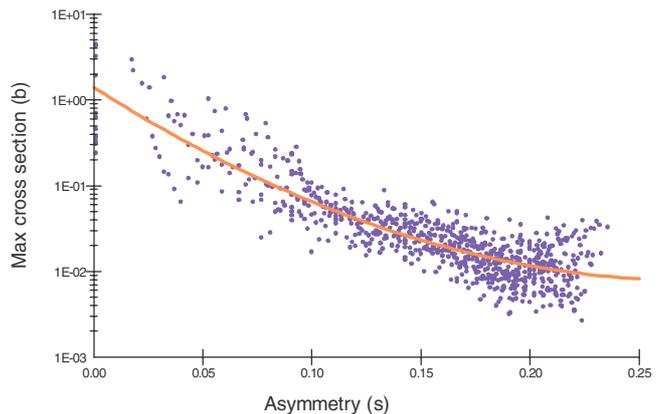


Fig. 7. $\sigma_{\text{max}}(s)$ for all (n,p) reactions in EAF-2007. Reactions with targets $A < 20$ are excluded.

entered into SAFEPQA-II. A plot of the C/E values for the $^{100}\text{Mo}(n,2n)^{99}\text{Mo}$ reaction is shown in figure 5. 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 indicating agreement of the library data with the measurements.

It is always necessary to also consider the differential data for the reaction; these are shown in figure 6. Note that experimental data extend 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-2005 validation 453 reactions were considered, of these 202 were classed as validated. A further 38 reactions which were split into ground and isomeric state showed good agreement for the sum, although the details

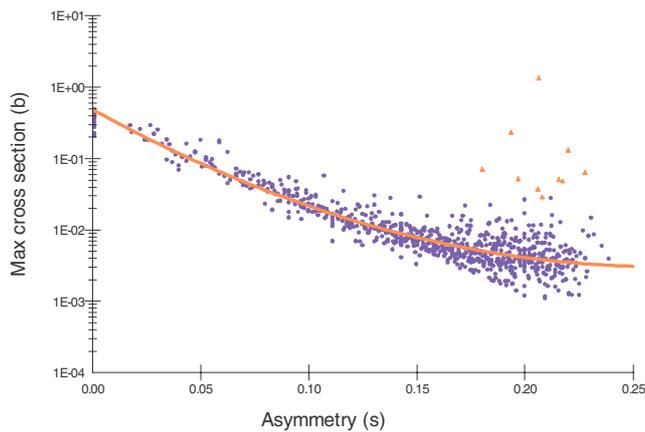


Fig. 8. $\sigma_{\max}(s)$ for all (n, α) reactions in EAF-2005. Reactions with targets $A < 20$ are excluded.

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.

4 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 the EASY-2005 validation there were 1,715 reactions with differential or integral data, so some other method is needed to test the majority of reactions. The method of Statistical Analysis of Cross Sections (SACS) has recently been developed [18]. 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 in the derivation of systematics. Similar effects have been seen for the maximum cross section (σ_{\max}). In SACS σ_{\max} , the energy of the maximum (E_{\max}) and the width at half maximum ($\Delta_{1/2}$) can be plotted as functions of A or s for all reactions of a particular type in the library. An example for (n, p) data in EAF-2007 is shown in figure 7.

Figure 7 shows a trend line and it can be seen that there is a well defined correlation, with 68% of the points lying within a factor of 1.78 of the curve.

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 figure 8 for (n, α) reactions, the very discrepant reactions around $s = 0.2$ are shown with a triangle symbol. The improvement of the (n, α) data in EAF-2007 can be seen by comparing figures 8 and 9.

5 Conclusions

The various parts of EASY-2007, such as the EAF data, are described. EAF-2007 contains deuteron- and proton-induced

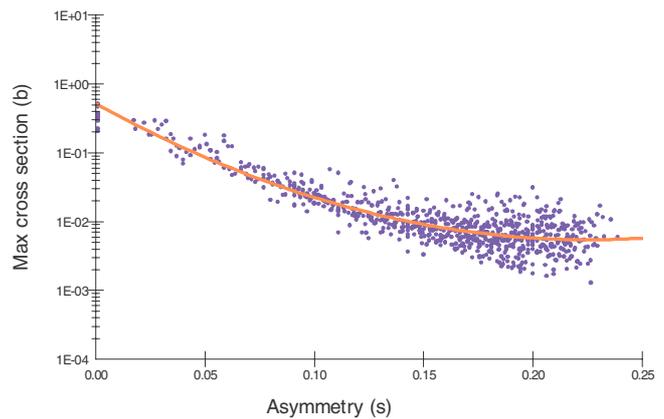


Fig. 9. $\sigma_{\max}(s)$ for all (n, α) reactions in EAF-2007. Reactions with targets $A < 20$ are excluded.

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.

This work, supported by United Kingdom Engineering and Sciences Research Council and the European Communities under the contract of Association between EURATOM and UKAEA, was carried out within the framework of the European Fusion Development Agreement. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

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