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The European Activation File: EAF-2001 cross section library

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Abstract

In the European fusion programme, safety and environmental issues are of great importance in the continuing development of power plants. In support of this programme, a sound, complete and reliable neutron cross section data library is required. The European Activation File (EAF) project has been an ongoing process performed through European and world-wide co-operation that has led to the creation of succeeding EAF versions. The latest release, EAF-2001, has benefited from the generation and maintenance of comprehensive activation files and the development of the new processing code SAFEPAQ-II. Cross section validation exercises against both experimental data and systematics, which were started on the EAF-4 files, enable a comprehensive assessment of the data. SAFEPAQ-II is used to apply a series of modifications to the original source data. A very important set of modifications concerns renormalisation and branching using experimental or systematic data. A total of 3,377 reactions have been so changed; 27% of all the reactions. These are challenging tasks when the source contains non-threshold reactions with an energy dependent branching ratio. Although EAF-2001 is the best-validated cross section library in the world, currently less than 16% of all the reactions can be compared with experimental information, and sometimes then only for very limited, and not always relevant, energy ranges.

As with EAF-99, results of integral experiments have been used to adjust data. For a small number of reactions this can be done using SAFEPAQ-II: the remaining integral data was compared with activation predictions made using EAF-99 and adjustment factors found. Validation using integral data has been performed by means of direct comparison with measurements of sample structural material under fusion-relevant neutron spectra. Irradiations have been carried out at ENEA FNG, FZK Isochron-cyclotron, Sergiev Posad SNEG-13 and JAERI FNS and integral C/E comparisons made (C/E is the ratio of the library to the experimental value). The results of these benchmarking exercises have indicated, in conjunction with differential data, where modifications to the data can be applied.

The EAF-2001 library contains 12,470 excitation functions involving 766 different targets from ^{1}H to ^{257}Fm, atomic numbers 1 to 100, in the energy range 10^{-5} eV to 20 MeV. The 1,700,000 lines that make up the pointwise file are then processed into numerous groupwise files with different micro-flux weighting spectra to meet various user needs. Uniquely, an uncertainty file is also provided that quantifies the degree of confidence placed on the data for each reaction channel.

Contents

Introduction

The European Activation File (EAF) is the collection of nuclear data that is required to carry out inventory calculations of materials that have been activated following exposure to neutrons. Along with the inventory code FISPACT [1], EAF comprises the European Activation System (EASY) which has been developed for fusion activation studies.

One of the components of EAF is the collection of neutron-induced cross section data. The present report documents this cross section library, detailing how the library has been developed over a fifteen year period, describing the methodology employed for its production and testing and providing an index of all the reactions. The present report forms part of the documentation for EASY, other reports cover the FISPACT code [1], SAFEPAQ-II [2] and other components of EAF [3,4,5].

The current release of the European Activation File, EAF-2001, contains cross section data of neutron-induced reactions for energies between 10^{-5} eV and 20 MeV. This report covers all the reactions. The library contains data for targets up to and including fermium (Z=100). A new version of the library has been produced by the SAFEPAQ-II tool, which uses data from various sources and applies a series of modifications. The choice of data sources and the basis of the modifications use the knowledge derived from previous EAF libraries as a starter. For EAF-2001 this starter knowledge was taken from the EAF-99 file [6]. This is the first time that SAFEPAQ-II has been used for library development rather than the SYMPAL/SAFEPAQ tools [7,8,9] that were used for previous versions. The change over from text based files to relational databases has been time intensive, but now that SAFEPAQ-II is in place future library development should be very efficient.

The new version contains the results of a sustained effort from many laboratories and physicists world-wide. The pointwise library has increased only slightly in size compared to the previous version (125 MB compared to 118MB), but has gained considerably in quality and completeness. All reactions with experimental data have been examined and reassessed where possible, while the experimental and systematics databases have been checked and expanded.

EAF-2001 contains data for 98 elements from H to Fm, but excludes data for the short-lived radioactive elements At and Fr. There are a total of 766 target isotopes, including ground, first and second isomers, which have non-zero cross sections (*i.e.* greater than 10^{-8} b) below an energy of 20 MeV. Cross sections to and from isomeric states are listed separately in a pointwise ENDF File 3 section format. This leads to a total of 12,470 reaction channels that contain data. During the creation of the library several checks were made to monitor the quality of the data. The procedures employed, forming a part of SAFEPAQ-II, are fully described in reference 2 and are summarised in Figure 1. The entire process is handled in an interactive fashion allowing new data to be input, existing data to be examined in graphical and tabular modes, modifications to be defined and validation carried out. All changes to data are automatically logged and this forms part of the quality assurance (QA) of the library.

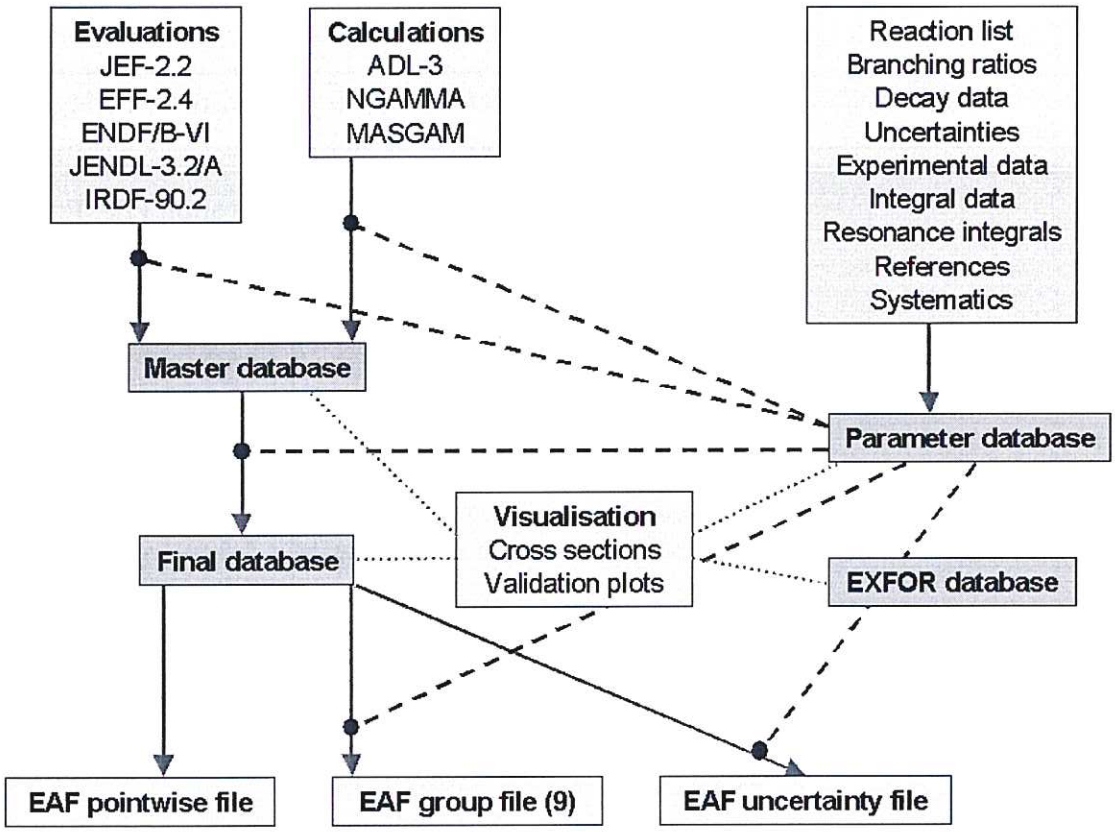

Figure 1. Flowchart of the SAFEPAQ-II processes. The arrows indicate flows of data, the dashed lines indicate that information in Parameter is required in the conversion and dotted lines show sources of data for visualisation.

Historical survey

EAF-2001 is the latest result of a large amount of work on activation data carried out world-wide. The present section puts it in its historical context, and enables references to some of this earlier work to be given. It is interesting that if we look back over the last 20 years and survey the questions that were being addressed by the fusion community about activation of materials in fusion devices and the tools available to give answers, it is evident that while the tools are much more extensive and sophisticated, many of the concerns are rather similar.

In the UK, the data library available for activation libraries was UKCTRIIIA, while the inventory code used was ORIGEN [10].

UKCTRIIIA was produced by Jarvis [11] from the earlier UKCTRIII [12]; both these libraries were designed for fusion activation calculations. UKCTRIIIA was a multigroup library (100 group GAM-II) that covered the energy range thermal - 15 MeV. It contained 1,477 reactions on 305 targets (note that U and Pu isotopes were included), some of which were radioactive (all radionuclides with $T_{½}$ > 10 days were considered as targets). It covered 10 reaction types, ((n,2p) and (n,n't) are the current reaction types missing). Reference 11 describes the data sources for the library, and while much of the library was from experimentally based sources, nearly 500 reactions were calculated by the simple model code THRESH [13]. The library contained isomeric states as daughters, but no long-lived isomeric states were included as targets.

In the early 1980s, ECN Petten (Netherlands) was involved in work, in collaboration with JRC Ispra, on the nuclear data needs for fusion activation. Collaboration between ECN and UKAEA lead to a new library UKCTRIII-AR2 [14] which contained renormalisation of a large number of the UKCTRIIIA cross sections to experimental data at 14.5 MeV [15] or to systematics. This library was used for a series of activation calculations, but it was recognised that it was far from complete (many stable nuclides were missing, and the radionuclides considered as targets was limited), based on simple model calculations and lacked a proper treatment of isomeric states.

In 1985 Mann *et al.* produced a new activation library - REAC [16]. This substantially increased the number of reactions to about 6,000 (although the number of targets remained at about 300). This US library was made available to ECN Petten (there was a tripartite collaboration between ECN, UKAEA and Hanford, starting in about 1986, which involved sharing of data

libraries). It should be noted that REAC was a pointwise library and that the data extended to 40 MeV. Another important difference from UKCTRIIIA was that reactions such as (n,t) and (n,n'd) which produce the same daughter nuclide were not lumped together. This is important if accurate calculations of gas production are to be carried out.

Library development was continued at ECN by the process of renormalisation of REAC and the addition of data for radioactive targets. The new library was named REAC-ECN-1 [17]. The main features of REAC-ECN-1 were:

- An additional comment line was included in REAC-ECN-1. Note that REAC had a single comment line; apart from these lines both files are in ENDF/B-5, MF=3 format. The MT reaction identifiers are adopted except that for production of isomeric states, 300 (for m) or 600 (for n) is added.
- The GAM-II group format file GREAC-ECN-1 is similar to that of UKCTRIIIA except for the addition of the two comment lines. There are additional reactions so the ENDF MT numbers have been adopted, and then multiplied by 10 and the state value of the daughter added.
- The aim was to include all radionuclides with $T_{½} > 1$ day as targets, in fact all the isomeric targets and a few ground state targets were missing.
- Data values at 14.5 MeV were compared with available experimental data, and renormalised if necessary.
- The branching ratios at 14.5 MeV were checked and if no reliable experimental data were available, the branching ratio was set to 0.5.
- Systematics at 14.5 MeV were taken from Qaim [18] and Kumabe and Fukuda [19]. These were used to renormalise the data from model calculations.

Further work followed at ECN leading to the release of REAC-ECN-2 [20]. This corrected some errors and introduced new systematics. The main features are :

- The systematics of Forrest [21] were adopted for production of charged daughters.
- The isomeric branching ratio was changed from 0.5 to a value determined by systematic formulae [22,23] that depend on the isomeric state spin of the daughter nuclide. Only in the case of (n,γ) reactions did the general value of 0.5 remain.

- Isomeric targets were included, these had the same cross sections as for the ground state.
- Some additional data sources were used for checking and renormalisation at 14.5 MeV.

The next library release by ECN was REAC-ECN-3 [24]. This contained 8,466 reactions in the energy range thermal to 20 MeV. Its main features were:

- Checking and improvement of 51 important reactions which produce long-lived radionuclides.
- Addition of 6 short-lived isotopes.

At about the same time a new library, UKACT1 [25,26], was produced by UKAEA. This was based on the same REAC library, but was only available in the GAM-II group structure. It used as a starter file GREAC-ECN-1, to which were added more targets (using THRESH) so that all radionuclides with $T_{½}$ > 1 day had data (in addition 34 nuclides with shorter half-life were included where a product formed by a single reaction is an important long-lived nuclide). Some features were:

- It included 49 first isomers and 4 second isomers as targets, and included all isomeric daughters with $T_{½}$ > 1s.
- All targets included capture reactions (although for some radionuclides these were estimated).
- Superelastic collisions were included (these refer to (n,n′) reactions from an isomeric state to the ground state).
- Checks were made to ensure that none of the standard reactions from each target were missing.
- UKACT1 contained 8,719 reactions on 625 targets.

By 1989 it was realised that it was unnecessary for such parallel library development at ECN and UKAEA to occur, so it was agreed that UKAEA would maintain the decay data library and the inventory code FISPACT, and that ECN would maintain the cross section library. UKAEA would continue to contribute to cross section development, but pass all data to ECN who would supply group libraries to UKAEA. By such collaboration an activation 'package' was developed.

This strategy led to the starter file for the European Activation File (EAF-0) [27], although it is also referred to as REAC-ECN-4 in some ECN reports. Note that this was also the first library that was assembled by the SYMPAL processing code (albeit an early version of SYMPAL with few of the features

found in the final version [8]). The main improvements in EAF-0 over REAC-ECN-3 were:

- Addition of reactions on 142 targets (many of them isomers), isomeric targets had thresholds correctly different from ground state target. All targets with $T_{½}$ > 1 day included, giving 10,787 reactions.
- (n,n′) reactions improved.
- (n,3n) cross sections near threshold adjusted.
- Renormalisation at 14.5 MeV improved.

EAF-1 (REAC-ECN-5) [28], was the first of the EAF series to be widely used in activation calculations following its release in March 1990. A clear statement of the EAF strategy is contained in a paper presented in late 1989 [29], the main points are:

1. Address the completeness of the library using the existing tools.
2. Provide the library with a simple but complete uncertainty file.
3. Carry out uncertainty estimation and sensitivity studies which will provide feedback on the quality of important reactions.
4. Wherever possible, improve the quality in general using more advanced model codes.

The main features of EAF-1 were:

- The number of targets was increased by demanding that all radionuclides with $T_{½}$ > 0.5 day had data.
- Improvement of low-energy data, particularly for the (n,γ) and (n,n′) reactions.
- Inclusion of an provisional uncertainty file for important reactions covering the energy range thermal to 20 MeV.
- Use of more high quality evaluated files (*e.g.* from the JEF libraries).
- Special evaluations for 101 important reactions [29] to both long- and short-lived nuclides included.

The main emphasis for EAF-2 [30,31,32], which was released in May 1991, was to carry forward the EAF-1 improvements with special emphasis on the (n,γ) reactions. The main features were:

- 11,855 reactions on 699 targets.

- Use of some data from the international dosimetry file IRDF-90.
- Use of error factors derived from systematics [21] to assess the uncertainties for most of the reactions.
- Use of new data for renormalisation at 14.5 MeV.
- Group libraries in both GAM-II (100 groups) and VITAMIN-J (175 groups).

EAF-3 [33,34] was released in May 1992, the main features were:

- 12,899 reactions on 729 targets.
- Addition of 60 targets in the actinide range (At - Cm), the cross section data including the fission channel.
- Uncertainty file for all reactions in a 1 group (threshold reactions) and 2 groups (non-threshold reactions) structure.
- (n,p) and (n,α) reactions with positive Q-values were inspected and revised in the thermal region.
- (n,2p) reactions calculated by THRESH were inspected and revised in the 14.5 MeV region.
- Use of more evaluated data (from EFF-2, ENDF/B-VI and JEF-2).
- Improvements in the (n,γ) data [35,36], including addition of the pre-equilibrium component at high energies if absent.
- Use of energy dependent isomeric branching ratios for (n,γ) reactions.
- Check of EAF values with experimental data at three energies (0.0253 eV, 30 keV and 14.5 MeV).

EAF-3.1 was released in mid 1993; apart from the correction of minor errors the cross section library remained the same as EAF-3, the major change was in the uncertainty file [37]. This was substantially improved, but the format remained the same.

EAF-4 [38] was released in March 1995, its main features were:

- 13,096 reactions on 734 targets.
- Addition of 25 higher actinide targets (Ra - Fm).
- Replacement of many of the data generated by THRESH with either new evaluations or superior calculations.
- Improvement of the capture reactions, especially the energy dependent isomer ratio.

- Additional comparison and renormalisation to experimental data at 14.5 MeV.
- Branching ratio systematics were improved for threshold reactions.
- Use of all available evaluated data from EFF-2.4, IRDF-90, JEF-2.2, ENDF/B-VI and JENDL-3 libraries. Use of data from the activation file ADL-3 [39].
- Special care was taken with the reactions identified as particularly important for the ITER project [40].
- The uncertainty file contained more information for (n,γ) and (n,f) reactions. These were given in three groups rather than the two groups used previously. More experimental uncertainties were used to replace the generic values adopted from systematics.
- The groupwise library was made available in two additional group structures - WIMS (69 groups) and XMAS (172 groups).
- The ability to calculate sequential charged particle reactions in FISPACT was due to new EAF libraries developed at FZK. See the FISPACT-2001 user manual [1] for details of these libraries.

EAF-4.1 [41] was released in June 1995. This version was the last processed at ECN Petten. It corrected various errors introduced into EAF-4.0 during processing. EAF-4.1 contained 12,976 reactions on 736 targets. Note that for distribution to users only the groupwise libraries are released, these only contained data for targets H - Cm, the higher actinide data only appearing in the pointwise library.

Work over the period 1995-1996 was devoted to the installation of SYMPAL at UKAEA and the further development of SYMPAL, SAFEPAQ and EAF that enabled the production of the IAEA FENDL/A-2.0 [42] library.

EAF-97 [43] was released in the summer of 1997. It contained data for 12,469 reactions on 766 targets. Many new data sources and experimental data [44-53] were used in its production. Special emphasis was put on improving the actinide data and the capture data [54]. However erroneous interpolation laws were spotted when comparing plots of ENDF against PENDF and pointwise against groupwise files [55]. It was decided to modify EAF-97 to correct the interpolation laws and EAF-97.1 was produced in January 1998. The corrections led to the modification of the interpolation law for 353 reaction channels in the point-wise file.

During the period 1998 - 1999, extensive data validation work was carried out. This contributed to the release of EAF-99 [6] at the beginning of 1999. It contained 12,468 reactions on 766 targets and while covering the same reactions as EAF-97.1 benefited from the large amount of integral data generated as part of the European Fusion Technology programme. About 750 reactions were significantly modified based on the integral data and experimental data from EXFOR. New data sources that were available include the Russian dosimetry file (RRDF) and helium production library (HEPRL-96) [56], individual evaluations from IRK Vienna [57] and data corrections from LANL [58].

General improvements in the $1/v$ region for non-threshold reactions, additional calculations using NGAMMA, review of the (n,f) reactions and improvement of the uncertainty file were also areas of improvement in EAF-99.

Beginning in 1998 work started on the development of a new data evaluation and processing tool. This was designed to replace SYMPAL and SAFEPAQ and to use modern computer technology. SAFEPAQ-II was designed from scratch using relational databases and interactive graphics. It runs on the various Windows operating systems and thus has the advantage of portability (it has been installed at JUKO Research and CEA Cadarache) and of an automatic logging system that enables good quality assurance (QA) to be achieved. It is based on the ideas of SYMPAL and SAFEPAQ, but extends them and makes them more robust. A stable version was available in 2000 and it has been used in the production of EAF-2001.

New data sources, experimental and integral data were all incorporated in SAFEPAQ-II and the system was developed and tested during 2000 – 2001; the outcome of this work, in respect of the neutron induced cross section library, is described in this report.

Calculational tools

The preferred source of cross section data is one of the evaluated files. However, for many nuclides (especially radioactive nuclides) no such source is available and cross sections must be calculated. The code THRESH [13] has been mentioned in the previous section and this was widely used in earlier versions. It is however, very unsophisticated and a wider range of tools are now preferred. Many of these (FISPRO, MASGAM [59], MASGAM+SIG-ECN and NGAMMA [60])

are applicable to (n,γ) reactions. NGAMMA is used widely in the production of EAF-2001 and is outlined below.

A simple model code that is very suitable for mass-production runs, EXIFON [61], has been used in recent EAF versions for the threshold reactions (n,2n), (n,3n), (n,p) and (n,α).

NGAMMA

NGAMMA is based on the spherical optical model, the Hauser-Feshbach formula with width fluctuation correction, the exciton model [62] and the unified model [63] in which equilibrium and pre-equilibrium emission mechanisms are unified and angular momentum conservation is taken into account. This exact treatment of pre-equilibrium processes replaces the approximation on systematics as applied in MASGAM. Besides the radiative capture channel the code also handles the competing particle emissions, including neutrons, protons and alphas. The possibility to renormalize the calculation to experimental data or to systematics is maintained.

The main input parameters are:

- **E1, M1 and E2 strength function models and giant resonance parameters**. The generalized Lorentzian formulation [64] has been adopted for the E1 resonance, except for deformed nuclei in the mass range above A = 150, for which the classical Lorentzian was used (based on conclusions in [65,66]). The giant E1 resonance parameters have been taken from [67] and checked against the very recent compilation of Varlamov [68]. If the experimental data on the E1 giant resonance were missing, the value from the neighbouring target have been extrapolated. The spin-flip M1 resonance has been adopted for M1 radiation with the standard parameterization [64], the cross section σ_0 has been renormalized against the systematics (for details see reference 60). The single-particle model is used for E2 radiation.

- **Optical model**. Standard global neutron optical model parameters of Moldauer [69], Wilmore-Hodgson [69], Buck-Perey [70,71] and M. Uhl [72] have been tested on several nuclei ranging from A = 90 - 205 and the parameters of Uhl, giving the best results, were finally adopted for calculations.

- **Discrete levels and level density**. Discrete levels have been taken from corresponding compilations published in Nuclear Data Sheets. The newly evaluated set of BSFG

(back shifted Fermi gas) level density model parameters of the Beijing group (recommended by the IAEA RIPL/CRP) [89] have been used. In cases where no data were available, an extrapolated estimate from systematics was applied.

The Master database

The library development tool SAFEPAQ-II contains several relational databases that contain data required in the construction of the EAF libraries. The Master database contains data for each required reaction taken from the original data sources, in cases where the reaction is split but the original data is for the total, the total is present for all the split reactions. The data thus require many modifications to be carried out systematically before they can be used in EAF. Each original data source was converted into a source database and it is the entries in the source databases that are selected and used in Master.

The sequence of modifications that are applied to Master in the process of producing the Final database are fully described in the User Manual [2]. These include the checking of Q-values and thresholds, identification of reactions with suspect interpolation laws and removal of data points above 20 MeV. The branching and renormalisation are largely automatic, using data in the tables of the Parameter database. This contains all the relevant decay data extracted from the EAF decay data library such as isomeric spins. Spins are required during the branching process and SAFEPAQ-II automatically ensures that these are consistent in the decay and cross section libraries.

The original data in Master are not changed in any way, all modifications are applied to a copy held in Final. This means that the Master data are available at any time to be visualised; they can be compared with EXFOR data, other data sources and with Final data as the various modifications are progressively applied. If a new data source is required for a particular reaction there are tools available in SAFEPAQ-II to change the source in Master, create the modifications and apply these to generate the Final data.

The Parameter database

The Parameter database contains all the information that describes a particular version of an EAF library. The list of reactions and their sources that are included in the library, the list of nuclides, their sources and properties and the set of experimental information that can be used to renormalise or split a particular cross section. These values are stored in a

series of tables that are described fully in reference 2, but the most important are listed below to show the range of data.

- Energy boundaries of the group schemes.
- Systematic branching ratios as a function of spin.
- Decay data for all nuclides.
- Systematic error factors for reaction types.
- Experimental data at 25.3 meV, 30 keV, 14.5 MeV.
- Integral data in various neutron spectra.
- Log of all data changes.
- Pre-modifications and modifications.
- List of nuclides contained in libraries.
- List of reactions contained in libraries.
- Literature references.
- Resonance integral data.
- Neutron spectra data.
- Cross section systematics.
- Summaries of data in Final.
- Uncertainty data.
- Nuclide masses from Wapstra.
- Known biological hazard, A_2 and clearance values.
- Details of progress of library processing.

14.5 MeV systematics

The SAFEPAQ-II code contains information on the systematic formulae at 14.5 MeV, these are listed below for reference.

In the formulae below, s is the asymmetry parameter of the target nuclide = $(N\text{-}Z)/A$ and all cross sections are in mb. Note that the (n,2p) formula is new for EAF-2001.

(n,p)

The systematics of Forrest [21] and Doczi et al. [73] are used:

$$\sigma_{np} = 7.657(A^{1/3}+1)^2 \exp(-28.80s - 59.24s^2 + 0.2365A^{1/2}) \quad Z \geq 40$$

$$\sigma_{np} = 23.659(A^{1/3}+1)^2 \exp(-23.041(s+s^2)) \quad Z < 40$$

(n,α)

The systematic of Majdeddin et al. [74] is used:

$$\sigma_{n\alpha} = 15.0678(A^{1/3}+1)^2 \exp(-27.55(s+s^2))$$

(n,d+n′p), (n,d) and (n,n′p)

The systematics of Forrest [21], Kopecky [75] and Qaim [18] are used:

For light nuclei: ($s \leq 0.125$)

$$\sigma_{nd} = 9.94\exp(-0.11s)$$
$$\sigma_{nnp+d} = 900.9(A^{1/3}+1)^2\{1-0.4828\tanh(\xi+1)\}\exp(-52.3s-135.7/A)$$
$$\sigma_{nnp} = \sigma_{nnp+d} - \sigma_{nd}$$

For heavy nuclei: ($s > 0.125$)

$$\sigma_{nnp+d} = 900.9(A^{1/3}+1)^2\{1-0.4828\tanh(\xi+1)\}\exp(-52.3s-135.7/A)$$
$$\sigma_{nd} = \sigma_{nnp+d}/14.25 \quad \text{if } \xi < 0$$
$$\sigma_{nd} = \sigma_{nnp+d}/2 \quad \text{if } \xi > 0$$

ξ is the difference between the proton and neutron separation energies. If this formula has a value less than or equal to zero then the following alternative is used:

$$\sigma_{nnp} = 0.1\sigma_{nd}$$

(n,t)

The systematic of Forrest [21] is used, note the units are μb:

$$\sigma_{nt} = \begin{cases} 1.516(A^{1/3}+1)^2\exp(-24.35s+0.2670A^{1/2}), & A \text{ even} \\ 4402.1\exp(-20.509s), & A \text{ odd} \end{cases}$$

(n,n′d)

An approximate value is used:

$$\sigma_{nnd} = 0.1\,\sigma_{nt}$$

(n,h)

The systematic of Lishan et al. [76] is used, note the units are μb:

$$\sigma_{nh} = 0.75(A^{1/3}+1)^2\exp(-11.338s)$$

(n,n′α)

An approximate value is used:

$$\sigma_{nn\alpha} = 0.125\,\sigma_{n\alpha}$$

(n,n')

The systematic of Vonach [23] is used. This is held as a table of values for various isomeric spins, and no analytic formula is presented.

(n,γ)

The systematic of Kopecky *et al.* [28] is used:

$$\sigma_{n\gamma} = 1.18 - 1.13\exp(-0.01338A)$$

(n,2n)

The systematic of Badikov *et al.* [77] is used:

$$\sigma_{n2n} = 47.015(A^{1/3}+1)^2(1-3.9777\exp(-24.116s))$$

(n,2p)

The systematic of Kopecky is used, note the units are μb:

$$\sigma_{n2p} = 48.49\exp(-2.99s)$$

This is a new systematic, the details of its derivation are presented here as there is no available reference. (n,2p) experimental data were extracted from EXFOR and are listed in Table 1. Due to difficulties in measuring such small cross sections and the competition with the (n,p) and (n,n'p) data in the (n,xp) channel, only a limited number of data are available, some of which are only upper limits.

Table 1. Experimental values of (n,2p) cross sections [μb] extracted from EXFOR.

Target	Q (MeV)	BR63	GR66	HU68	LU70	QA70,73	CS79
E (MeV)		14.7	14.7	14.8	14.6	14.7	14.7
Si-29	13.38	<500					
K-41	14.51	<130			<50		
Sc-45	11.1	<210			25±10		
Ti-50	16.64	<280			<100		
V-51	14.17	<30			60±59		
Mn-55	14.33	<300			<110		
As-75	11.49	<500			52±19		
Rb-87	15.46				<5		
Y-89	11.61	<30			50±40		
Nb-93	8.88	<500			50±20		
Tc-99	10.31					<14	
Rh-103	9.96		<3	10.6±6			
Cs-133	8.88	<5			25±20	<12	
La-139	10.86	<46			30±20		
Pr-141	8.20	<840					0.73±10
Tb-159	8.84	<80					

The data sources are:

BR63 – Bramlitt and Fink [78]
GR66 – Gray [79]
HU68 – Hussain [80]
LU70 – Lulic et al [81]
QA70 – Qaim [82]
QA73 – Qaim [83]
CS79 – Csikai and Chouak [84]

Figure 2 shows the data points and systematic fit (the very low point of Csikai is excluded). The data shows only a small dependence on the the asymmetry parameter and it is expected that a typical cross section value would be 10 – 100 μb. By contrast the EAF-99 data generally underestimate the experimental values by about two orders of magnitude, and therefore the use of the systematic in EAF-2001 makes a significant difference.

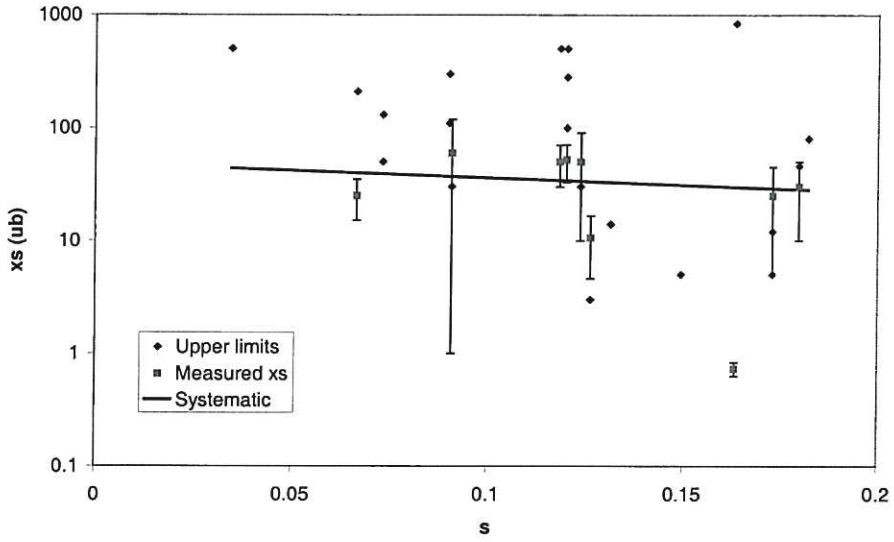

Figure 2. (n,2p) cross section showing fit of systematic formula.

30.0 keV systematics

The SAFEPAQ-II code contains information on the systematic formula at 30 keV for the (n,γ) reaction, this is a new systematic for EAF-2001 derived by Kopecky. It is shown below for reference. Details of its derivation are presented here as there is no available reference.

Introduction

Compilation [85] and measurements of capture cross sections at kT = 30 keV have been carried out by Kaeppeler. The cross section at this energy is an important quantity for astrophysical studies (nucleosyntheseis), in particular for the s-neutron capture process. The quoted values are Maxwellian averaged cross sections, in the case of approximately $1/v$ shapes the

$<\sigma_{30keV}>$ value is close to σ_{exp} (within 10%). This condition is also satisfied for unresolved resonance regions with a high density of resonances, and the values can be used as point-wise data. Data from reference 85 were collected in SYMPAL, but they were not used for any renormalisation purposes. Systematics have been derived from the dataset [86,87,59,35].

An update of the 30 keV data compilation has recently been completed at FZK and made available to us prior to publication [88]. This new compilation has been used to refine the systematics formula. The 30 keV cross section can be described by equation 1.

$$\sigma_{n\gamma} \approx ((2I+1)/D)\times\Gamma_{\gamma} \quad \text{.....(1)}$$

The first term in (1) corresponds to the level density (D is the average level spacing) and the second is the total radiative width. If the Fermi gas approximation for the level density is made (a is the level density parameter, U is the exitation energy and A is the mass number) and a standard parameterisation of Γ_{γ} is applied then equation (1) can be rewritten as equation (2).

$$\sigma_{n\gamma} \approx \exp(aU)^{1/2} \times AaU \quad \text{.....(2)}$$

Equation (2) can be simplified for a fit to the experimental data with 5 parameters as shown in equation (3).

$$\sigma_{n\gamma} = C_1 \exp C_2 (aU)^{1/2} \times A^{C_3} a^{C_4} U^{C_5} \quad \text{.....(3)}$$

This formulation has been used [87] for a limited data set, but it was shown [59,35] that the simplification to equation (4) using 2 parameters gives results of comparable accuracy.

$$\sigma_{n\gamma} = C_1 (aU)^{C_2} \quad \text{.....(4)}$$

Using values for a and U taken from the RIPL compilation [89] and data from reference 88 only for those targets with RIPL values and spliting the targets into odd and even Z enables Figures 3 and 4 to be plotted. The actual fitting parameters are shown below.

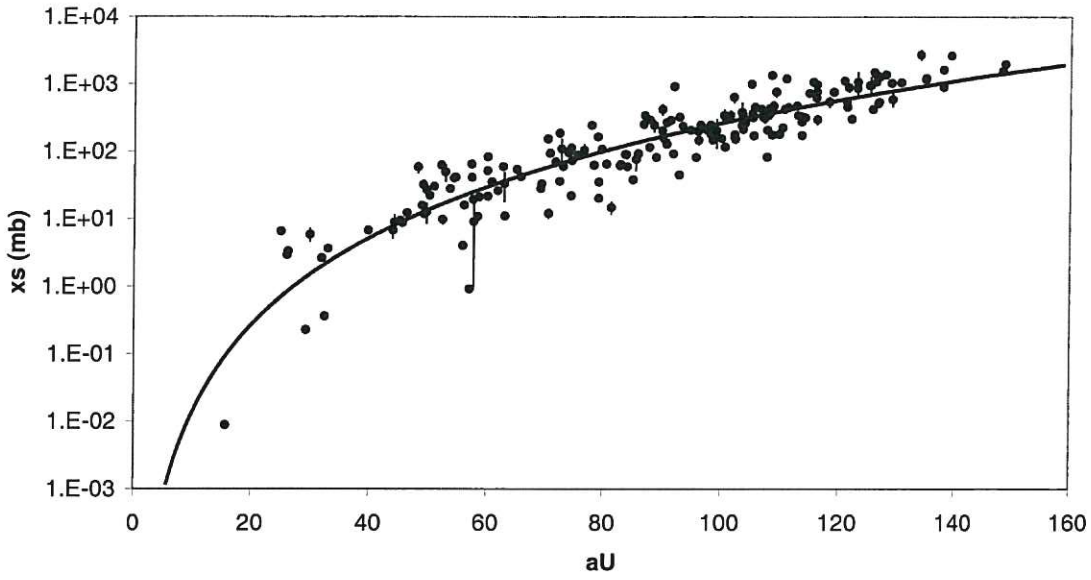

Figure 3. 30 keV cross sections for even Z targets showing fit of systematic formula.

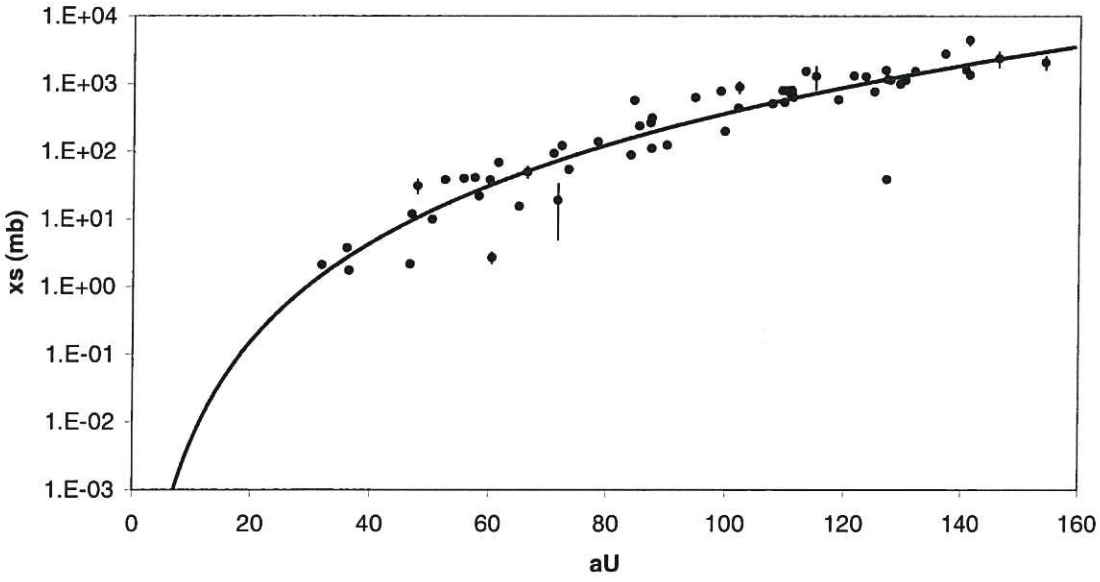

Figure 4. 30 keV cross sections for odd Z targets showing fit of systematic formula.

(n,γ)

The systematic of Kopecky is used:

$$\sigma_{n\gamma} = C_1(aU)^{C_2}$$

Values of a are stored in a table in the Parameter database for various values of neutrons (N). U is defined in terms of the Q-value and the pairing energies by $U = Q(n,\gamma) - P(Z) - P(N)$. The pairing energies are given in the same Parameter table. Values of the fitting parameters C_1 and C_2 depend on whether the number of protons (Z) is odd or even.

$C_1 = 8.236 \times 10^{-8}$, $C_2 = 4.827$ Z odd

$C_1 = 6.995 \times 10^{-7}$, $C_2 = 4.287$ Z even

Error factors

Related to the systematic formulae are values of the error factor (f) which quantify how well the systematic fits the experimental data. The error factor derived from the systematics is used in the generation of the uncertainty file if no experimental data are available. Table 2 lists the error factors used in SAFEPAQ-II.

Table 2. Error factors derived from systematics.

Reaction	Systematic	Error factor (f)
(n,n′)	Vonach [23]	2.0
(n,2n)	Badikov [77]	1.4
(n,3n)	Estimate	3.0
(n,4n)	Estimate	3.0
(n,n′α)	Estimate	3.0
(n,d)	Forrest [21]	3.0
(n,n′p)		2.0
(n,t)+(n,n′d)	Forrest [21]	1.6
(n,n′t)	Estimate	5.0
(n,n′h)	Estimate	5.0
(n,f)	Estimate	1.5
(n,γ)	Kopecky [28]	2.0
(n,p)	Forrest [21]	1.5
(n,h)	Lishan [76]	1.9
(n,α)	Madjdeddin [74]	1.6
(n,2p)	Estimate	3.0
(n,2α)	Estimate	3.0
(n,2n′p)	Estimate	3.0
(n,3n′p)	Estimate	3.0
(n,n′2α)	Estimate	3.0
(n,2n′α)	Estimate	3.0

Branching ratio

The splitting of a total cross section between isomeric daughters is a major data adjustment task carried out by SAFEPAQ-II. If at least two experimental values are available at 14.5 MeV (out of a total of three: σ_{tot}, σ_g and σ_m), then the branching ratio can be deduced and applied to the total cross section.

Table 3. Branching ratio ($b = \sigma_m/(\sigma_g + \sigma_m)$) as a function of the isomeric state spin (J_m).

J_m	Single-particle emission at 14.5 MeV	(n,γ) reaction at 0.0253 eV	Multi-particle emission at 14.5 MeV
0	1.90E-01	4.20E-01	1.40E-01
0.5	2.40E-01	5.00E-01	2.00E-01
1	3.10E-01	6.00E-01	3.10E-01
1.5	3.90E-01	7.00E-01	4.40E-01
2	4.80E-01	8.00E-01	6.00E-01
2.5	7.50E-01	7.50E-01	7.70E-01
3	6.70E-01	6.90E-01	7.50E-01
3.5	6.70E-01	4.90E-01	7.50E-01
4	6.40E-01	3.50E-01	7.20E-01
4.5	6.00E-01	2.50E-01	6.70E-01
5	5.20E-01	1.80E-01	6.20E-01
5.5	4.40E-01	1.30E-01	5.60E-01
6	3.80E-01	9.60E-02	5.00E-01
6.5	3.00E-01	6.20E-02	4.40E-01
7	2.20E-01	4.00E-02	3.90E-01
7.5	1.60E-01	2.50E-02	3.30E-01
8	1.10E-01	1.60E-02	2.80E-01
8.5	7.50E-02	1.00E-02	2.30E-01
9	5.00E-02	6.20E-03	1.90E-01
9.5	3.40E-02	3.80E-03	1.55E-01
10	2.20E-02	2.30E-03	1.15E-01
10.5	1.40E-02	1.50E-03	9.00E-02
11	9.00E-03	9.50E-04	6.70E-02
11.5	6.00E-03	6.30E-04	4.80E-02
12	4.00E-03	4.00E-04	3.40E-02
12.5	2.60E-03	2.40E-04	2.30E-02
13	1.70E-03	1.60E-04	1.60E-02
13.5	1.10E-03	1.00E-04	1.10E-02
14	6.80E-04	6.70E-05	7.80E-03
14.5	4.80E-04	4.20E-05	5.00E-03
15	3.00E-04	3.00E-05	3.30E-03
15.5	1.80E-04	1.80E-05	1.90E-03
16	1.20E-04	1.20E-05	1.00E-03
16.5	7.68E-05	7.58E-06	8.03E-04
17	4.93E-05	4.99E-06	5.09E-04
17.5	3.17E-05	3.25E-06	3.19E-04
18	2.04E-05	2.13E-06	2.00E-04
18.5	1.32E-05	1.39E-06	1.26E-04
19	8.47E-06	9.14E-07	8.08E-05
19.5	5.42E-06	5.81E-07	5.12E-05
20	3.52E-06	3.83E-07	3.35E-05

In cases where no experimental information on cross sections to ground or isomeric state is available, branching ratio systematics are used. The original systematics of neutron-induced isomer cross section ratios at 14.5 MeV [22], based on simplified GNASH calculations have been revised. This revision was based on recent experimental data and results of model calculations [90-92]. It is applied to all threshold reactions at 14.5 MeV. The new recommended values are listed in columns 2 and 4 of Table 3.

In order to account more accurately for the specificity of the branching ratio for radiative capture (thermal and resonance regions) and its strong energy dependence, the following approach has been adopted. Two branching ratios, one for the thermal and resonance range (b_L) up to energy E_H (end of resolved resonance range) and one for the high-energy range (b_H), have been adopted.

For the low-energy range all available experimental data at thermal energies were used and the derived branching ratio was assumed representative for this energy range. Further systematics have been derived from these data by a simple eye-guide procedure [93] and the recommended values are given in column 3 of Table 3.

For the smooth high-energy part, starting from the energy E_H, the systematics for one-particle emission in Table 3 have been used. The energy dependence of the branching ratio for (n,γ) systematics has been introduced in the following way. The value of b_L is kept constant up to E_H and then linear interpolation is used to connect with the b_H value at 14.5 MeV. This approach has been tested against a few rigorously evaluated branching ratios [90-92] with the code GNASH and there is reasonable agreement.

Q-values

The procedure which calculates the reaction Q-values and energy threshold uses data from the Audi-Wapstra mass-excess table [94]. This table covers 2655 nuclei and is supplemented with the Duflo-Zuker empirical mass formulae [95] when the nuclei did not exist in the table (for around 160 nuclei). It should be noted that SAFEPAQ-II generates Q-values and threshold energy modifications automatically. A total of 3758 such modifications are carried out, this represent 30% of the source evaluations.

EAF-2001 production

Data origin

EAF-2001 was generated starting with the information present in EAF-99. Because of the use of SAFEPAQ-II rather than SYMPAL/SAFEPAQ considerable time was spent ensuring that the databases contained information corresponding to EAF-99, and then this was used to generate libraries that agreed with the EAF-99. Data was then changed based on new sources and experimental data. The new data sources available were:

- Evaluations by IRK on ^{58}Ni and ^{60}Ni [96].
- Calculations by Mengoni [97] on light nuclides.
- Calculations using NGAMMA by Kopecky for a range of targets.

Summary of reaction types

It is useful to show how the reactions in the library can be divided into different categories; a number of relevant statistics are given in this section. Firstly, the data origin - the neutron cross sections included in EAF come from numerous sources having varying levels of quality and formats.

Table 4. Origin of data in EAF-2001.

Data Source	Number of reactions
ACTL	2
ADL-3	8428
ADL-3/I	12
BROND-2.2	1
CRP	8
CRP(MENGONI)	2
EFF-2.4	456
EFF-2.4(MDF)	4
ENDF/B-VI	60
ENDF/B-VI(MDF)	7
ESTIMATE	18
EXIFON	273
FEI	8
FENDL/A-1	34
FENDL/A-1(MDF)	1
FISPRO	9
HEPRL	29
IRDF-90.2	16
IRDF-P	4
IRK	41
JAERI	31
JAERI(MDF)	15
JEF-2.2	1953
JEF-2.2(MDF)	8
JENDL-3.1	161

Data Source	Number of reactions
JENDL-3.2	80
JENDL-3.2/A	77
JENDL-3.2/A/I	1
KOPECKY-2000	5
LANL	5
LANL(HERMAN)	13
LANL-2000	10
MASGAM	404
NGAMMA	23
SIG-ECN	1
SIGECN-MASGAM	64
THRES	206
Total	**12470**

It will be noted that in Table 4 some sources contain (MDF) in the label, e.g. JEF-2.2(MDF). Usually it is possible to reproduce data in EAF-99 by using the original data source and then applying the standard modifications. However, in a few cases changes have been made in previous EAF versions that are not fully documented. In these cases data have been extracted from the EAF-99 MDF (Master Data File).

Table 5. Reaction types in EAF-2001.

Reaction Type	Number of reactions
(n,2n)	1001
(n,3n)	861
(n,4n)	23
(n,γ)	1001
(n,f)	88
(n,n′)	256
(n,n′d)	895
(n,n′p)	917
(n,n′α)	897
(n,n′t)	785
(n,n′h)	208
(n,2p)	816
(n,2α)	2
(n,p)	1008
(n,d)	921
(n,α)	985
(n,t)	942
(n,h)	860
(n,2nα)	2
(n,2np)	1
(n,n2α)	1
Total	**12470**

The entire EAF-2001 reaction list is given in Appendix 4. It contains target and daughter state, data origin information, types of modifications and the number of data points for each reaction stored in the EAF-2001 pointwise file.

Secondly, the reaction types - 21 different reaction types can be found in EAF-2001 and these are listed in Table 5. All kinematically allowed reactions below 20 MeV are specified for each target isotope. These include threshold reactions as well as certain break-up channels on light nuclei. 766 target isotopes, for which all the major reaction types exist, are present in the file.

If new, *i.e.* short-lived or exotic, isotopes are to be included as targets, it is important to ensure that data are included for all the major channels. As a general rule including data for only a subset of the reaction channels is of limited use, and can lead to incorrect conclusions when used for inventory calculations.

EAF-2001 (n,γ) reaction

Improvements to the neutron capture data have been concentrated in the following areas:

- A number of standard improvements have been carried out, among them 1/v region renormalisation based on C/E data.

- The status of (n,γ) data for low A targets (A<20) has been reviewed by Mengoni, Kopecky and Shibata within the IAEA CRP on 'Photon production data' [98]. This was used extensively in the production of EAF-99. The theoretical basis for new calculations is based on the work of Mengoni [99]. It is recognised, that the Hauser-Feshbach statistical theory, which has been applied so successfully for medium and heavy-mass nuclei, cannot be used for light targets. Individual resonances (not always of a compound nature and the majority of them p-waves) and the 'background' s-wave and p-wave direct capture play an important role. Direct capture can be calculated theoretically, however cross sections with isolated resonances require experimental information since their parameters cannot be derived theoretically.

One new evaluation (^{9}Be), based on the Mengoni [97] calculations, has been adopted in EAF-2001 and several new calculations are in progress (*e.g.* ^{13}C, ^{17}O and ^{18}O).

- New calculations have been performed for 35 nuclei (e.g. ^{64}Zn, ^{80}Se, ^{82}Se, and ^{205}Tl), for which the previous MASGAM calculations resulted in a strange shape of the low energy part of the smooth statistical component. In order to improve these data, new calculations have been performed with the code NGAMMA. SAFEPAQ-II includes a

modification type to 'merge' high energy data from one source with the low energy data from the main data source. This is used to add the NGAMMA data in an interactive fashion.

It is useful to show how the (n,γ) reactions can be divided into different categories, and a number of statistics are given in this section. Firstly, the final states of the EAF-2001 (n,γ) reactions can be split as shown in Table 6.

Table 6. Numbers of different final states in EAF-2001.

Reaction	FS = 0	FS = 1	FS = 2	Total
(n,γ)	764	219	18	**1001**

Every target leads to an FS = 0 state. Note that there are 766 targets in the EAF-2001 library, however there are no (n,γ) reactions for ^{3}H and ^{7}Be. Hence a total of 764 target isotopes in the library undergo (n,γ) reactions. The (n,γ) cross section data are from a range of sources, and the number of reactions from each is shown in Table 7.

Table 7. The number of capture reactions from each data source in EAF-2001.

(n,γ) Data Source	Number of Reactions
ADL-3	7
BROND-2.2	1
CRP(MENGONI)	2
EFF-2.4	10
ENDF/B-VI	22
ENDF/B-VI(MDF)	2
ESTIMATE	1
FISPRO	9
IRDF-P	3
JAERI	2
JEF-2.2	363
JEF-2.2(MDF)	4
JENDL-3.1	43
JENDL-3.2	20
KOPECKY-2000	5
LANL	5
LANL-2000	10
MASGAM	404
NGAMMA	23
SIG-ECN	1
SIGECN-MASGAM	64
All	**1001**

The modifications applied by SAFEPAQ-II for the (n,γ) reactions cover many of the basic types. The numbers of each type of modification are shown in Table 8.

Table 8. Types of the modified (n,γ) reactions.

Modification	Number
Renormalise to systematics	77
Renormalise to experiment	19
Renormalise by a factor	454
Removes data points	13
Renormalise by linearly energy dependent branching ratio	446
Modification of *Q*-value	101
Change number of points	7
Pre-equilibrium addition	76
Change interpolation law	27
1/*v* addition	1
Add a data scrap	1
Data merge	69
Change energy value	696
Change cross section	1
Total (for 899 reactions)	**1988**

EAF evaluation tools

Different evaluation tools and model codes have been used earlier to generate the data that is lacking from the major evaluated data libraries available. They are: FISPRO, MASGAM and MASGAM + SIG-ECN and they are described in a previous report [54].

Recently several new evaluations have been performed using the code NGAMMA. The code NGAMMA [60] was adopted for fast calculations of (n,γ) cross sections in a similar way to MASGAM. Many input parameters (optical model parameters, level densities, gamma-ray strength functions) can be prepared from available global systematics or can be inputted manually using local parameters.

EAF-2001 actinide targets

The content of the EAF-2001 actinide sub-file includes 98 targets, ranging from ^{211}Rn up to ^{257}Fm. A number of corrections or data replacements have been performed for this version leading to a considerably improved data set of major reactions. All data have been thoroughly examined for their behaviour in two energy regions; thermal (1/*v* component) and the resonance region.

Data sources have been changed for several targets (^{231}Pa, ^{234}U, ^{236}Np, ^{240}Pu, ^{244}Cm, ^{247}Cm, ^{252}Cf, ^{254}Es and ^{254m}Es). A $1/v$ addition has been made for ^{239}Np and below E_H the cross section has been normalised to the thermal value.

The data sources and reaction types for the actinide targets are listed in Tables 9 and 10.

Table 9. Origin of actinide data in EAF-2001.

Data Source	Number of reactions
ENDF/B-VI	5
ESTIMATE	17
EXIFON	83
JAERI	29
JAERI(MDF)	15
JEF-2.2	134
JEF-2.2(MDF)	5
JENDL-3.1	86
JENDL-3.2	48
KOPECKY-2000	3
MASGAM	15
NGAMMA	14
THRES	144
Total	**598**

Table 10. Actinide reaction types in EAF-2001.

Reaction Type	Number of reactions
(n,f)	88
(n,γ)	98
(n,n′)	9
(n,2n)	95
(n,3n)	93
(n,4n)	23
(n,p)	96
(n,α)	96
Total	**598**

The resulting sub-file can certainly be claimed to be the most complete evaluated actinide data file available. The majority (76%) of the reactions have been modified in some way by SAFEPAQ-II.

EAF-2001 reaction nomenclature

A notation is adopted for describing reactions in the EAF library, the format of which is best illustrated by taking an example. Consider the (n,γ) reaction from a target of indium - ^{114m}In, which is initially in the first isomeric state and leads to a

final first isomeric state. The MASGAM code has been used to evaluate the cross section.

The two EAF title lines are:

```
IN*114N,G*     MASGAM
  |       |       |
  |       |       +-> data origin
  |       |
  |       +-> describes the FS
  |
  +-> describes the IS

MASGAM; ADJUST    [14, 4, 6, 3]
  |       |          |
  |       |          +-> modification codes
  |       |
  |       +-> first modification type
  |
  +-> data origin
```

IS (Initial State) refers to the target nuclide state, while FS (Final State) describes the state of the reaction product. Possible notations of the isomeric states are shown in Table 11.

Table 11. Notation of isomeric states.

Value (IS or FS)	EAF notation	State
0 or 99	-	Ground state or total
1	*	First isomer
2	#	Second isomer

Next the data source is given, which in the above example is MASGAM. A complete list of the data origins used to build the EAF-2001 library is given in Table 4, which identifies each source library or processing code which was used to calculate the cross section. The second line repeats the data source and then appends additional text to indicate further processing of the data. Currently the possible strings are:

- ; ADD (for Mod Type = 1, 11, 12, 16)
- ; SYST (for Mod Type = 2)
- ; EXP (for Mod Type = 3)
- ; RN (for Mod Type = 4, 6)
- ; DEL (for Mod Type = 5)
- ; QVALUE (for Mod Type = 7)
- ; NUM (for Mod Type = 8)
- ; PEQ (for Mod Type = 9)
- ; INT (for Mod Type = 10)
- ; MERGE (for Mod Type = 13)
- ; ADJUST (for Mod Type = 14, 15)

The SAFEPAQ-II User manual [2] gives more details of the Mod Type. ADD indicates that one or more data points have

been added (for example if Mod Type = 11 then a $1/v$ addition has been carried out). SYST indicates that a renormalisation to systematics has been carried out. EXP indicates that a renormalisation to experimental data has been carried out. RN indicates that a renormalisation has been carried out (for example if Mod Type = 6 then a linearly energy dependent branching ratio has been applied). DEL indicates that data points at high energy have been deleted. QVALUE indicates that the Q-value has been altered. NUM indicates that the number of data points at low energy has been changed. PEQ indicates that the Pre-equilibrium component (the direct capture) has been added to the cross section at high energies (usually important when E > 1 MeV). INT indicates that the interpolation law has been changed in an energy range. MERGE indicates that a second data source has been used at high energies and ADJUST means that energy or cross section value of a data point have been adjusted.

EAF-2001 modifications

SAFEPAQ-II carries out a large number of modifications (and pre-modifications), most automatically (dependent on the various flags set up in the Parameter database) but some through single reaction processing. The procedures carried out for branching are complex and are described in detail in the SAFEPAQ-II User manual [2]. Table 12 shows some statistics on the various modifications that are carried out. Note that reactions may have more that one modification.

Table 12. EAF-2001 modification numbers.

Mod Type	Number of Pre-mods	Number of Mods
1	0	0
2	72	580
3	0	308
4	0	2623
5	13	7787
6	0	446
7	423	3335
8	0	7215
9	76	0
10	0	1658
11	0	13
12	0	9
13	69	0
14	697	0
15	0	279
16	0	6927
Total	**1350**	**31180**

Table 13. EAF-2001 modifications classes.

Reactions	Number
Pre-modifications only	490
Modifications only	10346
Pre-modifications and modifications	644
Neither	990
Total	**12470**

Table 13 shows that only 990 reactions (7.94%) are completely untouched. This demonstrates that EAF-2001 does not simply combine in one file data that exist dispersed in others libraries, but does indeed significantly enhance those data that are important for activation and transmutation related applications.

EAF-2001 validation

EAF-2001 can be tested by the validation options in SAFEPAQ-II for consistency with the available experimental database or with predictions from systematics. Two main validation processes can be performed; one internal where comparison is performed against the database stored in the Parameter database and the other external where EAF-2001 excitation functions are compared either with EXFOR or other evaluated data files.

The EXFOR CD-ROMs are used by SAFEPAQ-II, data are selected from these and placed in the SAFEPAQ-II database EXFOR. It is from the latter that datasets can be displayed during visualisation. Considerable efforts have been to ensure that the EXFOR data selected are correct (daughter isomeric state and cross section units are two examples of checks). Checks of all reactions with EXFOR data have been made, and corrections made where appropriate.

Around 10% of the EAF-2001 library has been visually validated by comparing the excitation function with the experimental EXFOR database over the entire energy range. The EXFOR validation indicated reactions which required revisions. Two different ways of correcting the data have been applied:

- Replacement by a new evaluation (either from another source or a new calculation), in particular for cases with shape problems in the excitation function.

- Renormalisation of the whole or part of the excitation function through the interactive options available in SAFEPAQ-II.

A list of reactions that have been changed in response to this validation process is shown in Table 14.

Table 14. Details of changes in EAF-2001 following validation.

Reaction	Comment
$^{23}Na(n,\gamma)^{24g/m}Na$	Pre-equilibrium modification added, giving better agreement with experimental data.
$^{28}Si(n,p)^{28}Al$	The new data source ADL-3 was used to give better agreement with the experimental data.
$^{26}Mg(n,\gamma)^{27}Mg$	The new data source LANL-2000 was used to correct errors between 2-5 MeV.
$^{33}S(n,\alpha)^{30}Si$	A $1/v$ form of cross section added through the thermal experimental data.
$^{35}Cl(n,\alpha)^{32}P$	The new data source ADL-3 was used to give a more physical shape.
$^{36}Ar(n,\alpha)^{33}S$	The new data source JENDL-3.2/A was used.
$^{39}Ar(n,\gamma)^{40}Ar$	Renormalised above 10 keV, to agree with the 30 keV experimental value.
$^{46}Ca(n,\gamma)^{47}Ca$	Renormalised above 1.5 keV, to agree with the 30 keV experimental value.
$^{45}Sc(n,\gamma)^{46g/m}Sc$	The new data source JENDL-3.2 was used to give a better treatment of the resonances and better agreement with the experimental data.
$^{45}Sc(n,p)^{45}Ca$	The new data source JENDL-3.2/A was used to give a more physical shape.
$^{50}V(n,p)^{50}Ti$	Data renormalised to thermal experimental value below 1 MeV.
$^{51}V(n,n'p)^{50}Ti$	The new data source ADL-3 was used to give more physical high energy values.
$^{53}Cr(n,p)^{53}V$	The new data source ENDF/B-VI was used to give more physical high energy values.
$^{59}Cr(n,2n)^{58g/m}Co$	The branching ratio changed to give a better fit to the experimental data.
$^{61}Ni(n,\alpha)^{58}Fe$	The new data source ADL-3 was used to give more physical high energy values.
$^{64}Zn(n,\gamma)^{65}Zn$	NGAMMA data was used above 1 10^5 eV, agreeing well with the experimental data.
$^{68}Zn(n,p)^{68g/m}Cu$	The branching ratio changed to give a better fit to the experimental data.
$^{75}As(n,p)^{75}Ge$	The new data source ADL-3 was used to give better agreement with the experimental data at all energies.
$^{78}Se(n,p)^{78}As$	The new data source ADL-3 was used to give much better agreement with the experimental data at all energies.
$^{80}Se(n,\gamma)^{81g/m}Se$	NGAMMA data was used above 6.7 keV, agreeing better with the experimental data.
$^{82}Se(n,\gamma)^{83g/m}Se$	NGAMMA data was used above 31.1 keV, agreeing well with the experimental data.
$^{79}Br(n,\gamma)^{80g/m}Br$	NGAMMA data was used above 412 eV, agreeing well with the experimental data.
$^{81}Br(n,\gamma)^{82g/m}Br$	NGAMMA data was used above 3.63 keV, agreeing well with the experimental data.
$^{78}Kr(n,\gamma)^{79g/m}Kr$	Pre-equilibrium modification added.
$^{79}Kr(n,\gamma)^{80}Kr$	Renormalised above 13 eV, to agree with the 30 keV experimental value.
$^{81}Kr(n,\gamma)^{82}Kr$	Renormalised above 15 eV, to agree with the 30 keV experimental value.
$^{82}Kr(n,\gamma)^{83g/m}Kr$	Added pre-equilibrium modification. Renormalised below 100 eV to thermal experimental values. Changed the interpolation law to 5 between 1 – 51 keV.
$^{86}Rb(n,\gamma)^{87}Rb$	Renormalised above 47 eV, to agree with the 30 keV experimental value.
$^{87}Sr(n,n')^{87m}Sr$	Renormalised to give better fit to experimental data.
$^{88}Sr(n,\gamma)^{89}Sr$	The new data source JENDL-3.2 was used to give a better treatment of the resonances.
$^{90}Sr(n,\gamma)^{91}Sr$	A new evaluation (Kopecky-2000) made using NGAMMA. This also agrees much better than EAF-99 with the thermal experimental data.
$^{89}Y(n,\gamma)^{90g/m}Y$	The new data source LANL-2000 was used to correct errors above 0.15 MeV.
$^{90}Zr(n,p)^{90g/m}Y$	The new data source ADL-3 was used to give much better agreement with the experimental data at all energies.
$^{90}Zr(n,\alpha)^{87g/m}Sr$	The new data source HEPRL was used to give more physical high energy values.

Reaction	Comment
$^{90}Zr(n,n'\alpha)^{86}Sr$	The new data source HEPRL was used to give more physical high energy values.
$^{91}Zr(n,p)^{92g/m}Y$	The new data source ADL-3 was used to give much better agreement with the experimental data at all energies.
$^{91}Zr(n,\alpha)^{88}Sr$	The new data source HEPRL was used.
$^{91}Zr(n,n'\alpha)^{87g/m}Sr$	The new data source HEPRL was used.
$^{92}Zr(n,\alpha)^{89}Sr$	The new data source HEPRL was used to give better agreement with the experimental data.
$^{92}Zr(n,n'\alpha)^{88}Sr$	The new data source HEPRL was used.
$^{94}Zr(n,\gamma)^{95}Zr$	NGAMMA data was used above 42.45 keV, agreeing better with the experimental data.
$^{94}Zr(n,\alpha)^{91}Sr$	The new data source HEPRL was used to give better agreement with the experimental data at all energies.
$^{94}Zr(n,n'\alpha)^{90}Sr$	The new data source HEPRL was used.
$^{96}Zr(n,\alpha)^{93}Sr$	The new data source HEPRL was used to give better agreement with the recent experimental data.
$^{96}Zr(n,n'\alpha)^{92}Sr$	The new data source HEPRL was used.
$^{95}Nb(n,\gamma)^{96}Nb$	Data renormalised to thermal value below 1 keV.
$^{99}Tc(n,\gamma)^{100}Tc$	The new data source JENDL-3.2 was used to give a better treatment of the resonances.
$^{108}Pd(n,\gamma)^{109g/m}Pd$	NGAMMA data was used above 3.2 keV, agreeing better with the experimental data.
$^{108}Pd(n,2n)^{107g/m}Pd$	The new data source ADL-3 was used to give better agreement with the experimental data.
$^{108}Pd(n,p)^{108g/m}Rh$	The new data source ADL-3 was used to give more physical high energy values.
$^{109}Ag(n,\gamma)^{110g/m}Ag$	Pre-equilibrium modification added.
$^{106}Cd(n,\gamma)^{107}Cd$	The new data source ENDF/B-VI was used to give a better treatment of the resonances. NGAMMA data was used above 690 eV, agreeing better with the experimental data.
$^{110}Cd(n,\gamma)^{111g/m}Cd$	NGAMMA data was used above 7.16 keV, agreeing better with the experimental data.
$^{111}Cd(n,\gamma)^{112}Cd$	NGAMMA data was used above 2.32 keV, agreeing better with the experimental data.
$^{112}Cd(n,p)^{112}Ag$	The new data source ADL-3 was used to give better agreement with the experimental data.
$^{113}Cd(n,\gamma)^{114}Cd$	NGAMMA data was used above 300 eV, agreeing better with the experimental data.
$^{113}Cd(n,p)^{113}Ag$	The new data source ADL-3 was used to give better agreement with the experimental data.
$^{114}Cd(n,\gamma)^{115g/m}Cd$	NGAMMA data was used above 3.41 keV, agreeing much better with the experimental data.
$^{116}Cd(n,\gamma)^{117g/m}Cd$	NGAMMA data was used above 2.89 keV, agreeing better with the experimental data.
$^{113}In(n,n')^{113m}In$	Renormalised to give better fit to experimental data.
$^{114m}In(n,\gamma)^{115}In$	NGAMMA data was used above 2.15 eV, to agree with the 30 keV experimental value.
$^{115}In(n,2n)^{114g/m}In$	The branching ratio changed to give a better fit to the experimental data.
$^{114}Sn(n,\gamma)^{115}Sn$	The new data source JENDL-3.2 was used to give a better treatment of the resonances and thermal value. NGAMMA data was used above 2.5 keV, agreeing better with the experimental data.
$^{115}Sn(n,\gamma)^{116}Sn$	NGAMMA data was used above 693 eV, agreeing much better with the experimental data.
$^{116}Sn(n,\gamma)^{117g/m}Sn$	NGAMMA data was used above 2.15 keV, agreeing better with the experimental data.
$^{117}Sn(n,\gamma)^{118}Sn$	The new data source JENDL-3.2 was used to give a better treatment of the resonances. NGAMMA data was used above 611 eV, agreeing better with the

Reaction	Comment
	experimental data.
$^{118}Sn(n,\gamma)^{119g/m}Sn$	NGAMMA data was used above 1.89 keV, agreeing better with the experimental data.
$^{118}Sn(n,\alpha)^{115g/m}Cd$	The new data source ADL-3 was used to give better agreement with the experimental data.
$^{119}Sn(n,\gamma)^{120}Sn$	NGAMMA data was used above 547 eV, agreeing much better with the experimental data.
$^{124}Sn(n,\gamma)^{125g/m}Sn$	NGAMMA data was used above 6.5 keV, agreeing much better with the experimental data.
$^{124}Te(n,\gamma)^{125g/m}Te$	NGAMMA data was used above 5.7 keV, agreeing much better with the experimental data.
$^{133}Cs(n,\alpha)^{130g/m}I$	The new data source ADL-3 was used to give better agreement with the experimental data.
$^{137}Cs(n,\gamma)^{138g/m}Cs$	NGAMMA data was used above 10.6 keV, although there are no EXFOR data.
$^{134}Ba(n,\gamma)^{135g/m}Ba$	NGAMMA data was used above 2.07 keV, agreeing better with the experimental data.
$^{138}Ba(n,p)^{138g/m}Cs$	The new data source ADL-3 was used to give better agreement with the experimental data.
$^{139}La(n,t)^{137g/m}Ba$	The new data source ADL-3 was used to give better agreement with the experimental data.
$^{134}Ce(n,\gamma)^{135g/m}Ce$	NGAMMA data was used above 70 eV, to agree with the 30 keV experimental value.
$^{135}Ce(n,\gamma)^{136}Ce$	NGAMMA data was used above 10 eV, to agree with the 30 keV experimental value.
$^{140}Ce(n,\gamma)^{141}Ce$	NGAMMA data was used above 20 keV, agreeing better with the experimental data.
$^{140}Ce(n,p)^{140}La$	The new data source ADL-3 was used to give better agreement with the experimental data.
$^{141}Ce(n,\gamma)^{142}Ce$	The experimental 30 keV value was used to correct the cross section in the range 500 eV– 9 MeV.
$^{142}Ce(n,\gamma)^{143}Ce$	NGAMMA data was used above 4.88 keV, agreeing better with the experimental data.
$^{142}Ce(n,2n)^{141}Ce$	The new data source ADL-3 was used to give better agreement with the experimental data.
$^{143}Nd(n,2n)^{142}Nd$	The new data source ADL-3 was used to give a more physical cross section.
$^{144}Nd(n,2n)^{143}Nd$	The new data source ADL-3 was used to give better agreement with the experimental data.
$^{144}Nd(n,p)^{144g/m}Pr$	The new data source ADL-3 was used to give a more physical cross section.
$^{145}Nd(n,\gamma)^{146}Nd$	NGAMMA data was used above 2.17 keV, agreeing slightly better with the experimental data.
$^{145}Nd(n,2n)^{144}Nd$	The new data source ADL-3 was used to give a more physical cross section.
$^{146}Nd(n,2n)^{145}Nd$	The new data source ADL-3 was used to give better agreement with the experimental data.
$^{148}Pm(n,\gamma)^{149}Pm$	Data renormalised below 0.29 eV to thermal experimental value.
$^{149}Pm(n,\gamma)^{150}Pm$	NGAMMA data was used above 20 eV, to agree with the 30 keV experimental value.
$^{147}Sm(n,2n)^{146}Sm$	The new data source ADL-3 was used to give a more physical cross section.
$^{150}Sm(n,2n)^{149}Sm$	The new data source JENDL-3.2 was used to give better agreement with the experimental data.
$^{152}Sm(n,2n)^{151}Sm$	The new data source JENDL-3.2 was used to give better agreement with the experimental data.
$^{153}Sm(n,\gamma)^{154}Sm$	NGAMMA data was used above 4.7 eV, to agree with the 30 keV experimental value.
$^{151}Eu(n,3n)^{149}Eu$	The new data source ADL-3 was used to give better agreement with the experimental data.
$^{152}Eu(n,\gamma)^{153}Eu$	The new data source ENDF/B-VI was used to give a better treatment of the

Reaction	Comment
	resonances, renormalisation at high energy gives better agreement with the experimental data.
^{152m}Eu(n,γ)^{153}Eu	Data are renormalised to the thermal experimental value below 61.5 eV.
^{155}Gd(n,2n)^{154}Gd	The new data source JENDL-3.2 was used to give better agreement with the experimental data.
^{156}Gd(n,2n)^{155}Gd	The new data source JENDL-3.2 was used to give better agreement with the experimental data.
^{160}Gd(n,γ)^{161}Gd	NGAMMA data was used above 2.88 keV, agreeing better with the experimental data.
^{160}Dy(n,γ)^{161}Dy	NGAMMA data was used above 24.4 eV, agreeing much better with the experimental data.
^{162}Dy(n,γ)^{163}Dy	NGAMMA data was used above 430 eV, agreeing much better with the experimental data.
^{164}Dy(n,γ)^{165}Dy	NGAMMA data was used above 272 eV, agreeing much better with the recent experimental data.
^{166}Er(n,γ)$^{167g/in}$Er	NGAMMA data was used above 2 keV, agreeing better with the experimental data.
^{168}Er(n,2n)$^{167g/m}$Er	The branching ratio changed to give a better fit to the experimental data.
^{175}Lu(n,2n)$^{174g/m}$Lu	The new data source ADL-3 was used to give much better agreement with the experimental data.
^{177m}Lu(n,γ)$^{178g/m}$Lu	The experimental resonance integral was used to correct the cross section in the range 1 x 10^{-5} eV – 6.9 MeV by a factor 1.74 x 10^{-3}.
^{176}Hf(n,γ)$^{177g/m/n}$Hf	NGAMMA data was used above 1.28 keV, agreeing much better with the experimental data.
^{178}Hf(n,p)$^{178g/m}$Lu	The new data source ADL-3 was used to give better agreement with the experimental data.
^{180m}Ta(n,γ)^{181}Ta	NGAMMA data was used above 101 eV, to agree with the 30 keV experimental value.
^{181}Ta(n,2n)^{180}Ta	The new data source ADL-3 was used to give better agreement with the experimental data.
^{182}W(n,α)$^{179g/m/n}$Hf	The new data source ADL-3 was used to give better agreement with the experimental data.
^{184}W(n,p)^{184}Ta	The new data source ADL-3 was used to give better agreement with the experimental data.
^{190}Os(n,p)$^{190g/m}$Re	The new data source ADL-3 was used to give better agreement with the experimental data.
^{191}Os(n,γ)$^{192g/m}$Os	NGAMMA data was used above 15 eV, to agree with the 30 keV experimental value.
^{190}Pt(n,γ)^{191}Pt	NGAMMA data was used above 37.3 eV, to agree with the 30 keV experimental value.
^{193}Pt(n,γ)^{194}Pt	NGAMMA data was used above 15 eV, to agree with the 30 keV experimental value.
^{194}Pt(n,γ)$^{195g/m}$Pt	The new data source LANL-2000 was used to correct errors above 961 eV.
^{196}Pt(n,γ)$^{197g/m}$Pt	The new data source LANL-2000 was used to correct errors above 2.0 keV.
^{196}Pt(n,p)$^{196g/m}$Ir	The new data source ADL-3 was used to give better agreement with the experimental data.
^{198}Pt(n,γ)$^{199g/m}$Pt	The new data source LANL-2000 was used to correct errors above 1.58 keV.
^{197}Au(n,2n)$^{198g/m/n}$Au	The new data source IRDF-90.2 was used to agree better with experimental data.
^{201}Hg(n,γ)^{202}Hg	The new data source LANL-2000 was used to correct errors above 748 eV.
^{203}Tl(n,γ)^{204}Tl	NGAMMA data was used above 24.2 keV, agreeing better with the experimental data.
^{205}Tl(n,γ)^{206}Tl	NGAMMA data was used above 72 keV, agreeing much better with the experimental data.
^{231}Pa(n,γ)^{232}Pa	The new data source JENDL-3.2 was used to give a better treatment of the resonances and the data at high energies.

Reaction	Comment
^{237}U(n,f)	The new data source JENDL-3.2 was used to give a better treatment of the resonances and to agree with experimental data at high energy.
^{239}Np(n,f)	The data were renormalised below 30 keV to agree with the thermal experimental data.
^{243}Am(n,γ)$^{244g/m}$Am	The new data source ENDF/B-VI was used to give a better treatment of the cross sections at high energy.
^{244}Cm(n,γ)^{245}Cm	The new data source JENDL-3.2 was used to give a better treatment of the cross sections above 1 keV.
^{249}Bk(n,γ)^{250}Bk	The new data source JENDL-3.3 was used to give a better fit to the experimental data. A Pre-equilibrium modification was made.
^{250}Cf(n,f)	The data were renormalised below 200 keV to agree with the thermal experimental data.
^{253}Cf(n,γ)^{254}Cf	A new evaluation (Kopecky-2000) made using NGAMMA. This also agrees much better than EAF-99 with the thermal experimental data.
$^{254g/m}$Es(n,γ)^{255}Es	A new evaluation made using NGAMMA. This also agrees better than EAF-99 with the thermal experimental data.

The results of integral experiments have also been used to adjust data. Validation of activation code predictions, and thereby of the cross section and decay data, has been carried out by means of direct comparison with measurements of sample structural material under fusion-relevant neutron spectra. Having access to a variety of sources has allowed the energy dependence of the analysis to be very complete. Materials samples were irradiated in a wide range of simulated D-T neutron fields at JAERI FNS, Sergiev Posad SNEG-13, FZK Isochron-cyclotron and ENEA FNG, and different responses such as neutron spectra, emission spectra, kerma, activity and decay heat have been measured, allowing direct comparison with the code predictions [100-115].

The results of the different validation exercises, combined with other sources of information, led to a set of corrective actions to be carried out on some important reactions. These have been implemented in EAF-2001, and include cross section renormalisation, shape correction in a given energy range, threshold and *Q*-value correction, partial cross section adjustment and some new energy-dependent isomeric branching ratios. The fact that these benchmarks were performed by several research institutions using different activation codes and decay data has allowed clarification of the reasons for many discrepancies. These have been found to be partly due to inaccurate decay data, partly to inaccurate cross section data, and partly to a variety of inadequate calculational processes.

Figures 5 - 9 show examples of the types of modification that have been made for reactions in EAF-2001.

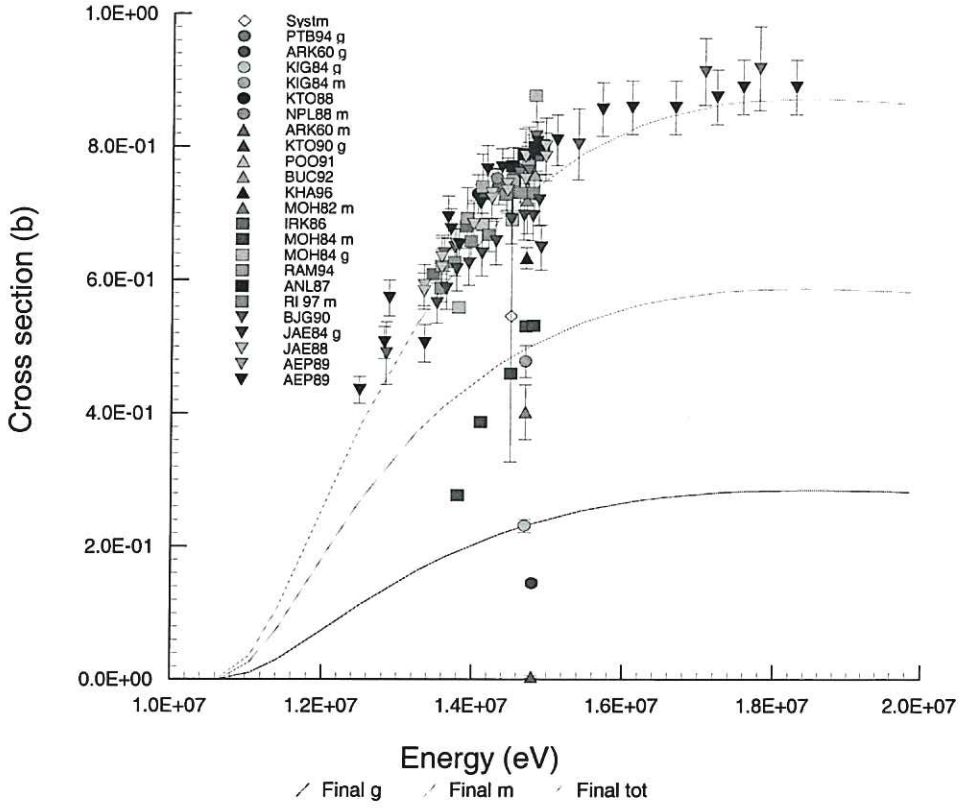

Figure 5. EAF-2001 plot for $^{59}Co(n,2n)^{60g/m}Co$.

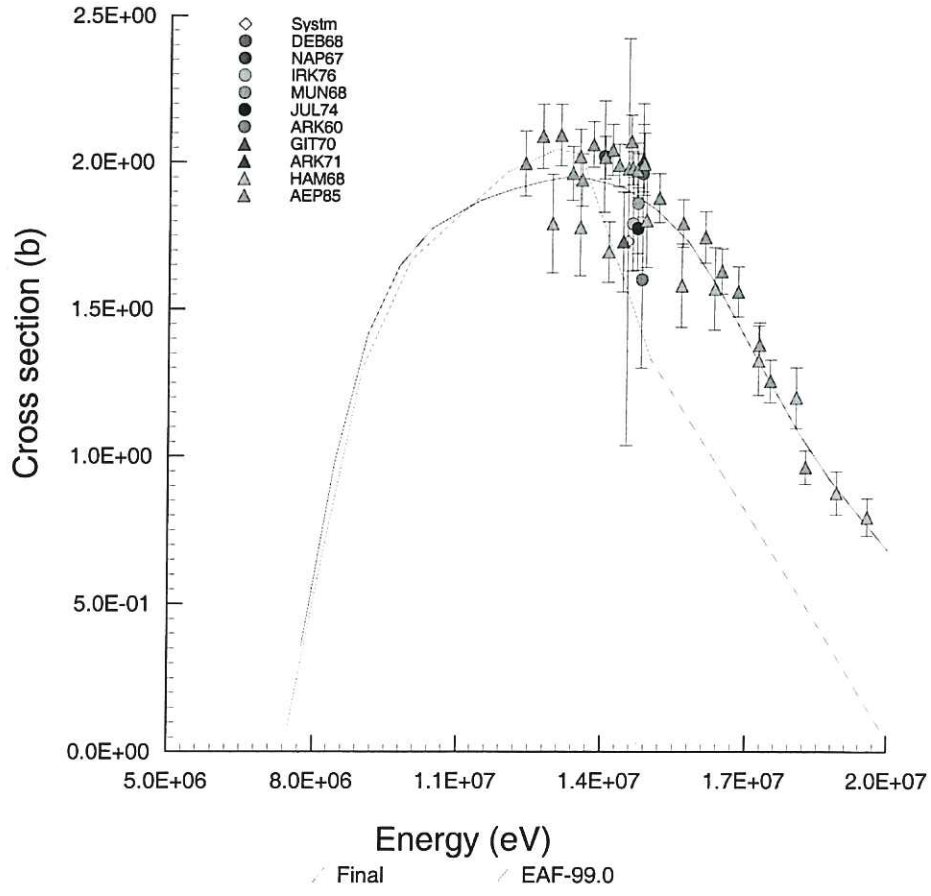

Figure 6. Comparison of EAF-2001 and EAF-99 plots for $^{142}Ce(n,2n)^{141}Ce$.

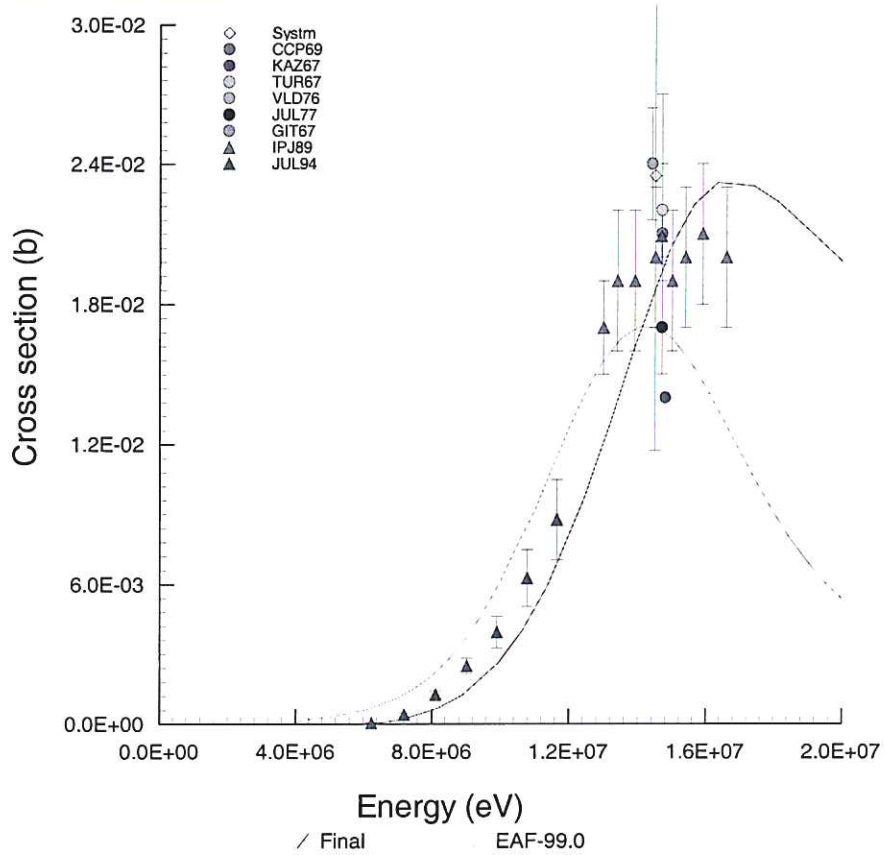

Figure 7. Comparison of EAF-2001 and EAF-99 plots for $^{78}Se(n,p)^{78}As$.

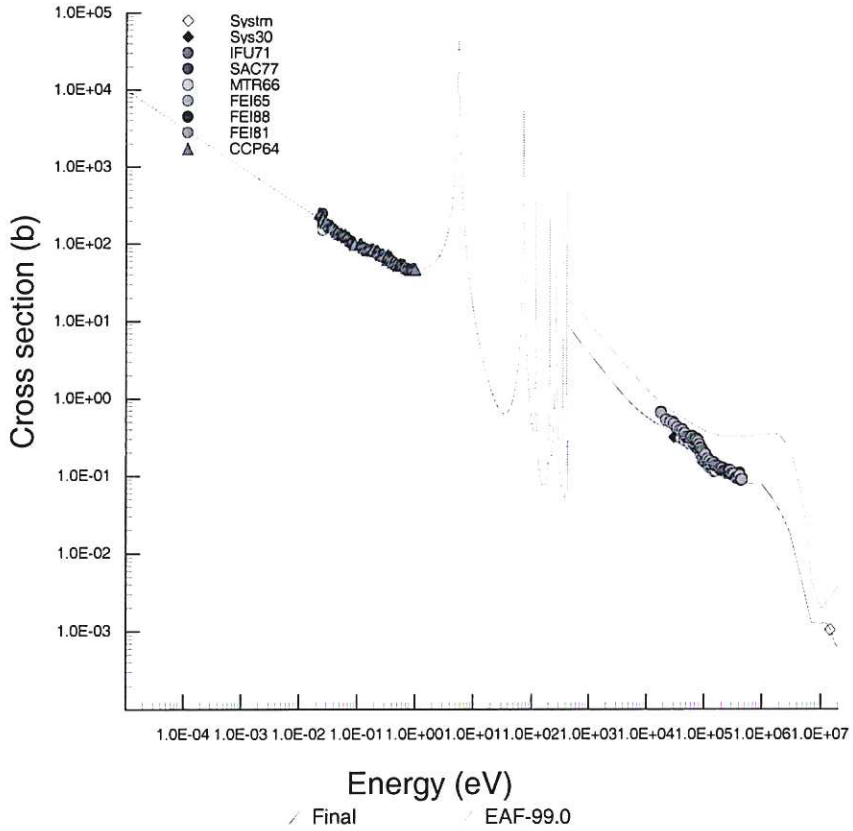

Figure 8. Comparison of EAF-2001 and EAF-99 plots for $^{162}Dy(n,\gamma)^{163}Dy$.

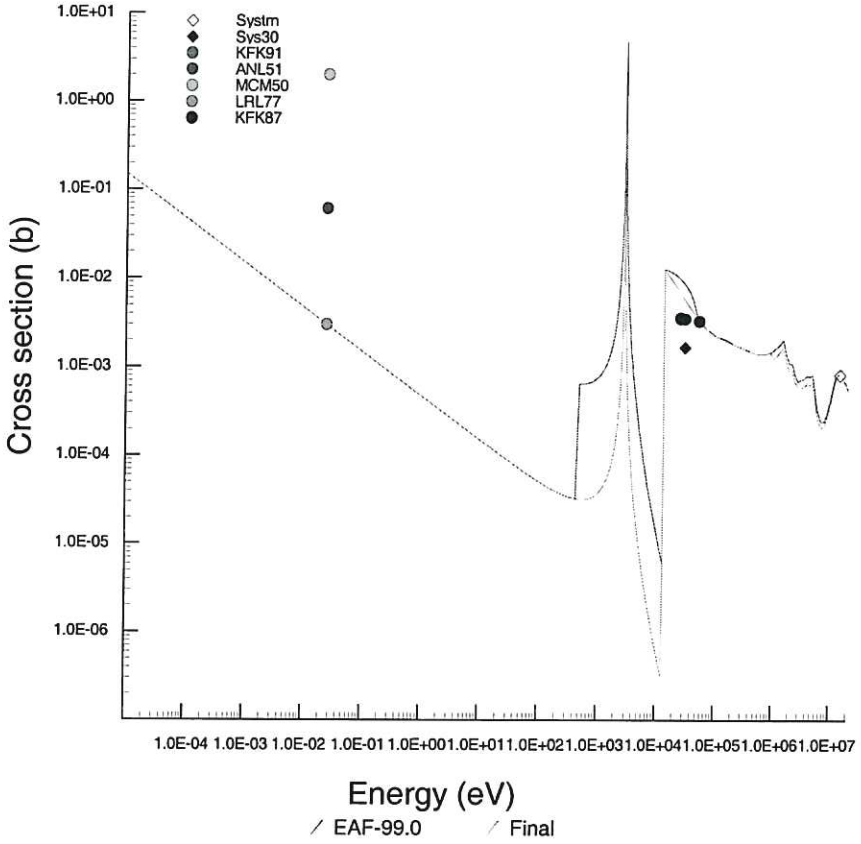

Figure 9. Comparison of EAF-2001 and EAF-99 plots for $^{86}Kr(n,\gamma)^{87}Kr$.

In Figure 5 the branching of a reaction into two final states is shown, there is considerable EXFOR data available for the two final states and the total, and this has lead to a change of the branching ratio from EAF-99. In Figures 6 and 7 it can be seen that EXFOR data has guided the change of data source so that EAF-2001 gives a very good fit to the experimental data. In Figure 8 NGAMMA data have been used at high energy (note the good fit to EXFOR data and to systematics at 14.5 MeV). In Figure 9 it can be seen that the renormalistion to the thermal experimental value has been carried out in a better way (energies up to 13 keV rather than 500 eV) in EAF-2001, giving a more physical shape to the single resonance.

Experimental validation - cross section

The experimental data available for selected cross section channels at three energy ranges, 14.5 MeV, 30 keV (for (n,γ) reactions) and 0.0253 eV held in the Parameter tables can be compared with the values in Final leading to the corresponding C/E values (C refers to the library value and E to the experimental data). These are plotted for the various reaction channels. Figures 10 - 15 present a selection of results from such a comparison. This process is an interactive one, thus the data in the file have been corrected using feedback from the early comparisons. This method presents clear advantages:

criteria can be set to decide when to applied a renormalisation process and trend analysis indicates certain deficiencies that can be related to either the raw data or their treatment in SAFEPAQ-II.

The (n,γ) experimental validation results are presented separately due to their importance and specificity. Such comparisons are made at thermal energy, 30 keV and at about 14.5 MeV and are based on a compilation of many references [9,35,46,49,59,116,117,118]. An ideal C/E ratio would clearly be 1, but in practice there is a distribution of C/E about this value. The number of C/E ratios available (flagged to be used for validation) for testing EAF-2001 is shown in Table 15.

Table 15. Number of (n,γ) experimental values available for each final state. FS = 99 indicates a total cross section.

FS	Thermal	30keV	14.5Me	Total
99	353	249	48	**650**
0	96	3	0	**99**
1	100	32	0	**132**
2	7	1	0	**8**
Total	**556**	**285**	**48**	**889**

A histogram may be formed from the distribution of C/E values, and plots at each energy for the (n,γ) reactions are shown in Figures 10 to 12. The numbers of C/E values shown on the graphs do not exactly agree with Table 15, this is because where ever possible if a reaction is split (FS=99 is not in the library), then the total has been formed and compared to experimental data for the total. Thus the same experimental data value can be used more than once.

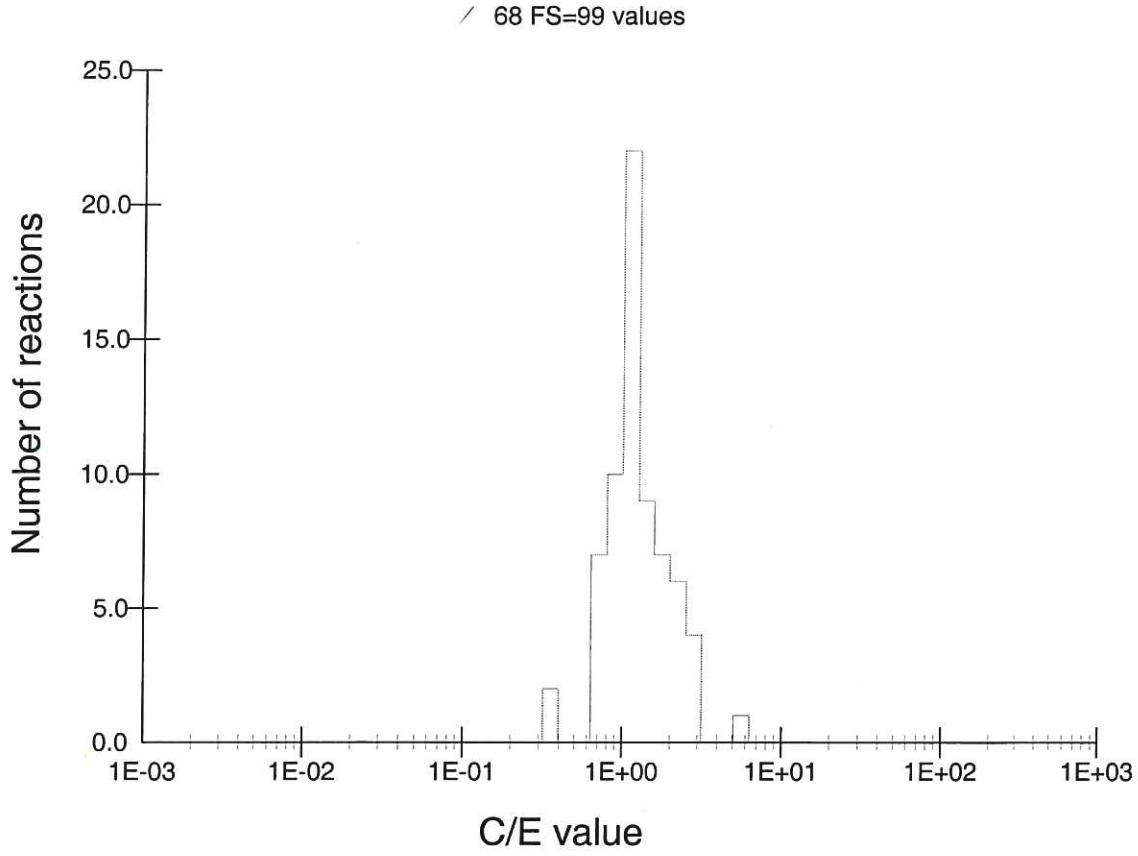

Figure 10. C/E distribution at 14.5 MeV for (n,γ) in EAF-2001.

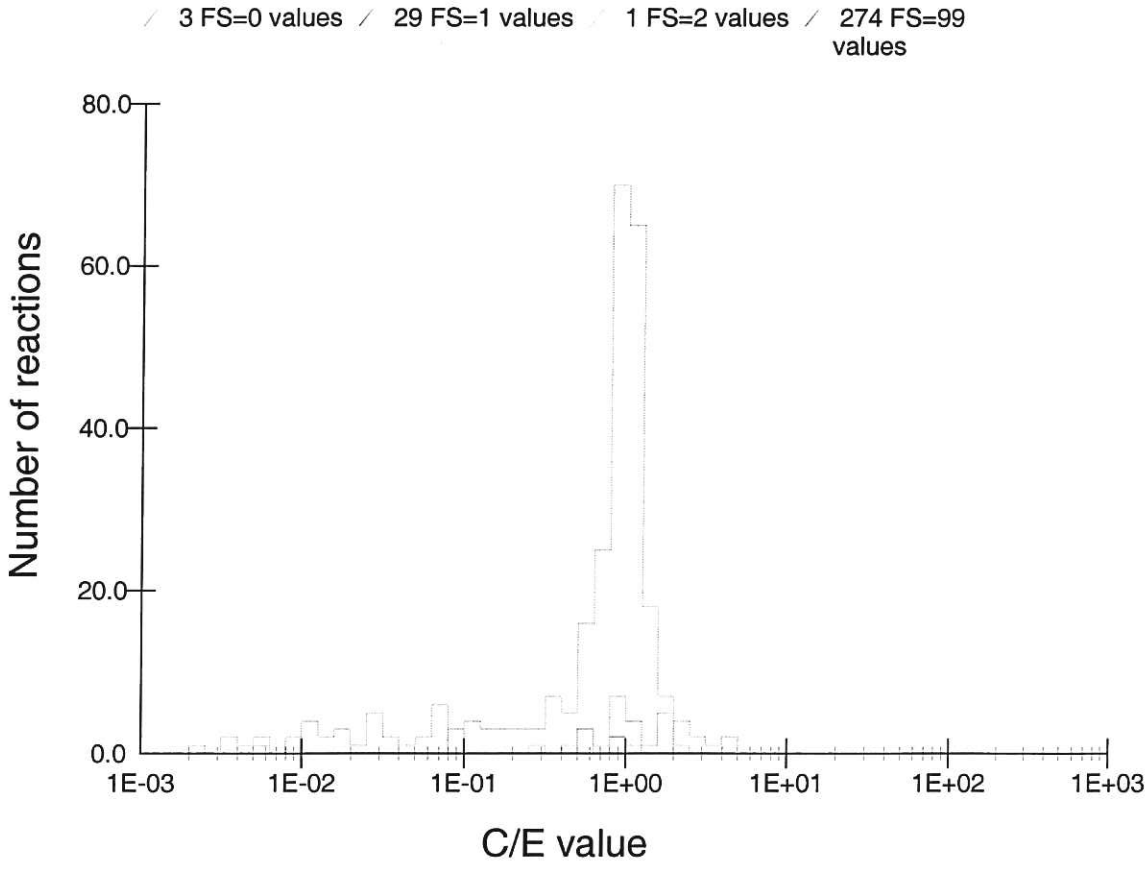

Figure 11. C/E distribution at 30 keV for (n,γ) in EAF-2001.

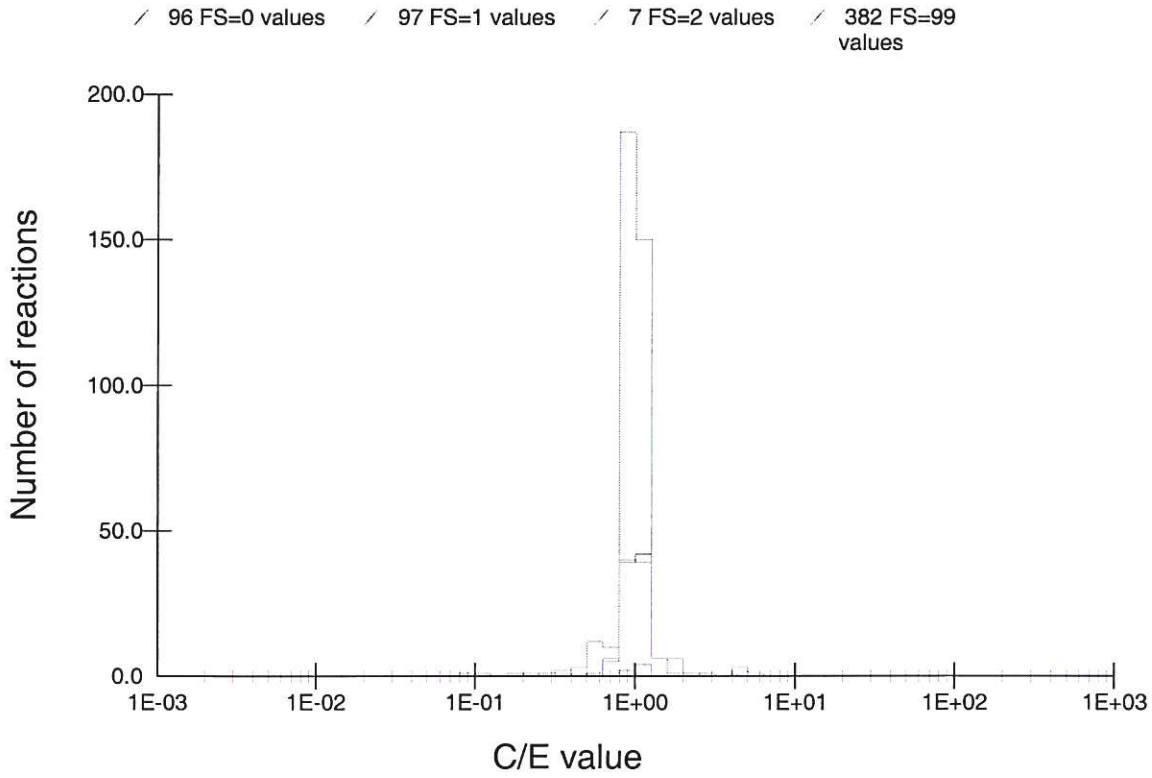

Figure 12. C/E distribution at 0.0253 eV for (n,γ) in EAF-2001.

Figures 10 to 12, show generally close agreement between the experimental values and the EAF-2001 data, with most C/E values close to a value of 1. This confirms the high quality of the (n,γ) cross section data available in the EAF-2001 library. Some small C/E values may be noted in Figure 11, they tend to be for nuclides which have a resolved resonance region around 30 keV. However, from such figures one can also note that 73% of the data can be compared with existing experimental measurements at thermal energy, 37% can be compared at 30 keV and only 6% at the energy range particularly important for fusion applications: 14.5 MeV.

It is clear from Figure 13 that the amount of experimental data available at 14.5 MeV (for all reactions) is rather limited, representing only 11% of the reactions. It is rather interesting to note from Figure 15 that some fission reaction are still not that well known, but it is fair to say that they belong to a set of rather unimportant fissionable nuclides.

These plots in conjunction with those presented earlier clearly demonstrate the state of the experimental data base today. However, since only 16% of all EAF-2001 reactions can be compared with experimental information, this indicates that both more experimental effort is required and that activation libraries also need to be compared to other quantities as described in the following section.

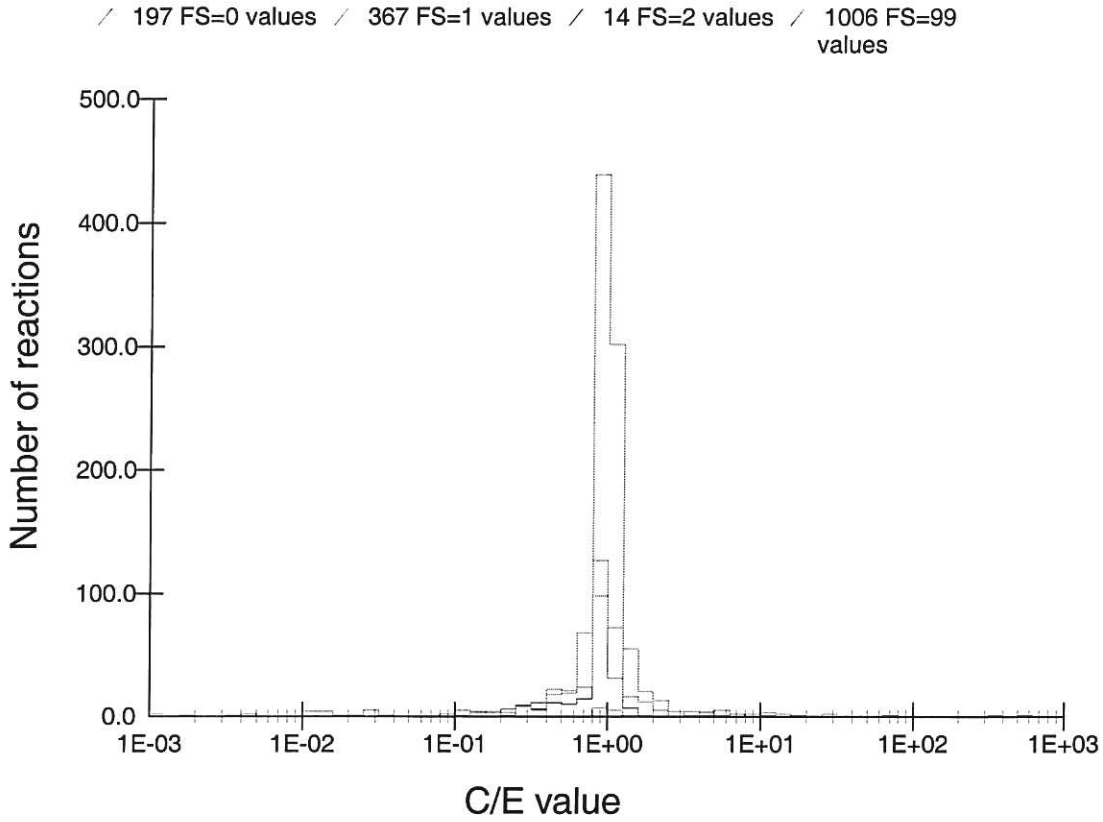

Figure 13. C/E distribution at 14.5 MeV for all reactions in EAF-2001.

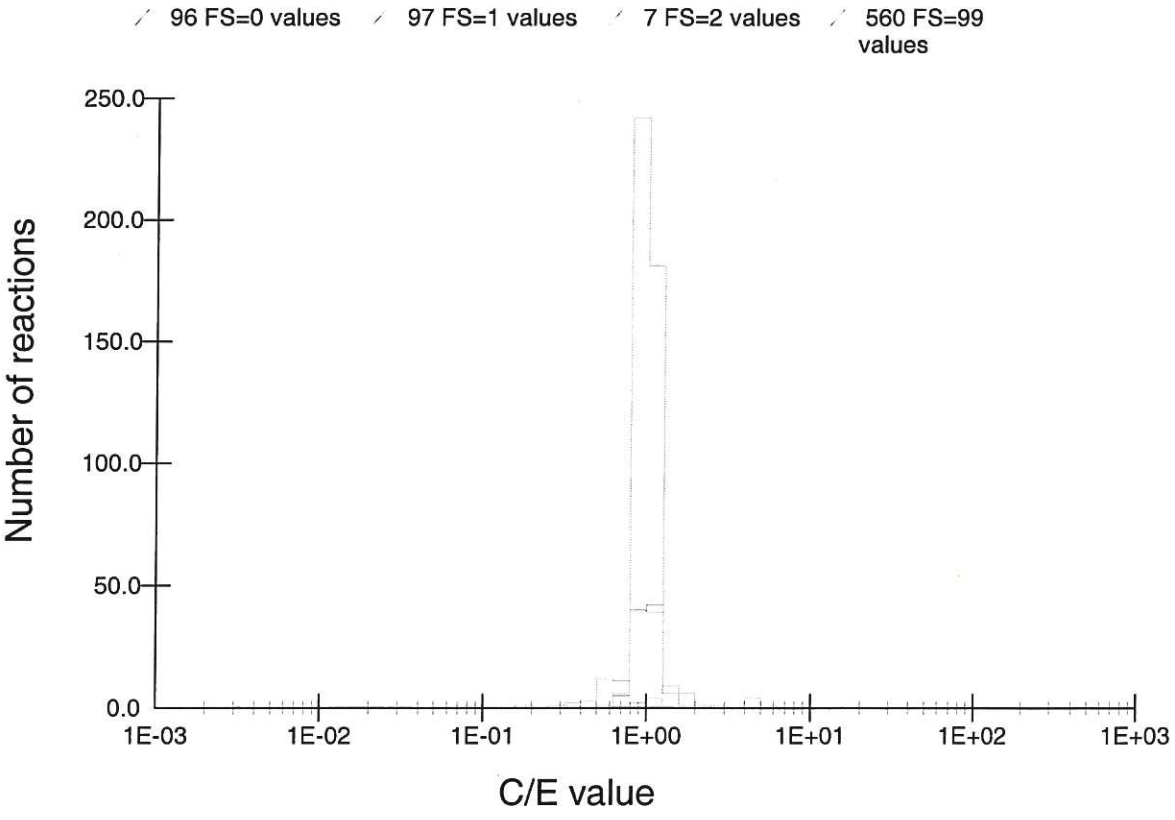

Figure 14. C/E distribution at 0.0253 eV for all reactions in EAF-2001.

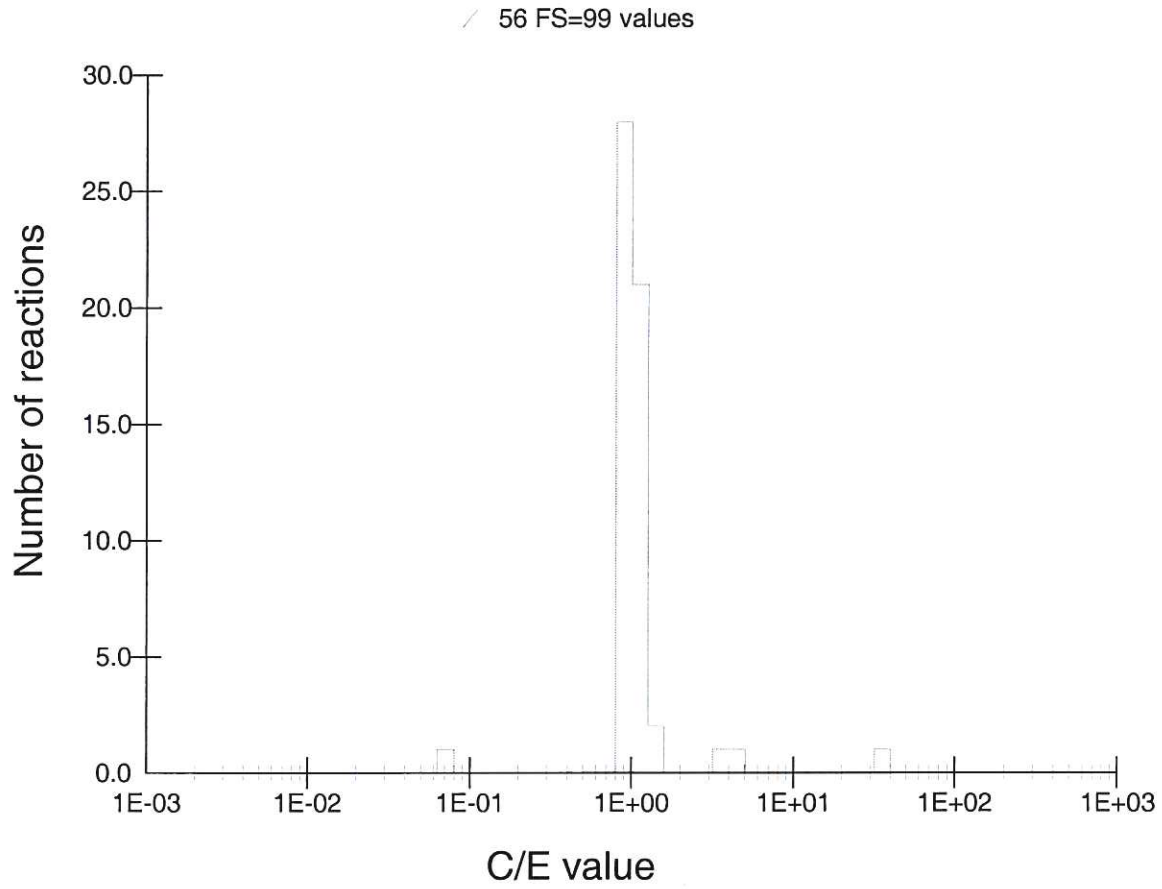

Figure 15. C/E distribution at 0.0253 eV for (n,f) in EAF-2001.

Experimental validation - resonance integral

Another very important experimental validation process can be carried out on the resonance integrals of certain reactions channels. To calculate the resonance integral the EAF-2001 data are Doppler broadened to 300 K and the integration limit of the integral is set from 0.5 eV to 100 keV. Such a validation allows a clear assessment of the quality of the cross sections profile over a wide energy range. The experimental data base is, however rather sparse with many deficiencies. One example is when the (n,p) and (n,γ) channels, which both count as absorption, simultaneously exist over the entire energy range and so contribute to the depletion term often given in experimental compilations. Figure 16 shows the C/E distribution for resonance integrals.

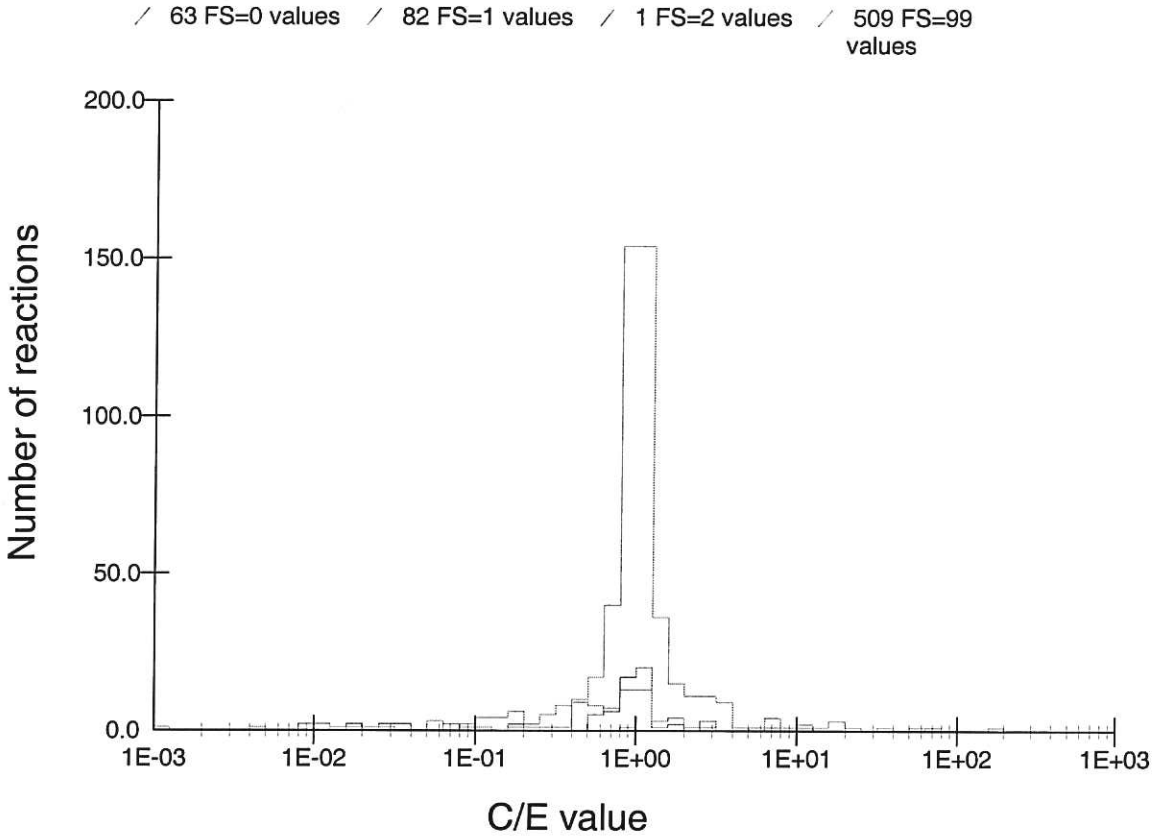

Figure 16. C/E distribution of resonance integrals in EAF-2001.

This validation is, however an important aspect of the qualification of the data for the (n,γ), (n,f), (n,p) and (n,α) channels. From an examination of these C/E values, it is planned to adjust the cross sections shape for those reactions where the discrepancies are large and the resonance parameters are not known in a future version of EAF.

Systematic validation

The predictions from systematics available for selected cross section channels at 14.5 MeV, can be compared with the values contained in the processed file leading to corresponding C/S values (C refers to the library value and S to the systematics prediction). Figures 17 - 26 present the results of the comparison for EAF-2001. The same analysis of the individual reaction channels, that was carried out for the experimental validation, can be applied here. Comparison with systematic predictions can be carried out for many channels, however, certain limitations do apply: the energy range is limited to 14.5 MeV, only total cross section C/S value can be compared, the validity of the formulae used may not cover the complete mass range and systematic formulae do not always account for competing reactions.

This clearly indicates that if one want to use information derived from C/S validation procedures, say for renormalisation, then one has to proceed with caution. This information does evidently present some advantages but the limitations described earlier tend to make its general implementation difficult.

From Figure 17, where all the C/S values are presented, one can immediately deduce the broad coverage, with 66% of the reactions compared. This in itself is quite an achievement and tends to demonstrate the rather satisfactory behaviour of the systematic formulae. It is important to keep in mind here that the same data, but in lesser number, have been previously compared with experimental information.

Figures 24 and 25 representing the C/S values for the (n,n′α), and (n,n′p) reactions, clearly demonstrate the difficulties encountered in applying systematic formulae for these reactions. Differences of about an order of magnitude can commonly be spotted that highlight less than satisfactory library contents. However, those are not major reactions and it has been shown by inventory calculations, that they are of importance only in a small number of particular cases.

At this stage it is important to keep in mind that even if certain cross sections are known to high accuracy in a particular energy range then it is not uncommon to find that comparison of the data with either evaluated files, experimental or systematic information at other energies can still generate significant discrepancies.

A comparison can be made at 14.5 MeV against (n,γ) systematics [35]. At this energy systematics formulae can be applied with some success, which is quite fortunate in view of the lack of information that exists in the experimental data base. Figure 26 clearly demonstrates that when a histogram of C/S values is plotted for all the 764 (n,γ) total cross sections, 74% of the data are within the range 0.8 - 1.25. The second peak at around 2 to 3 on the abscissa, (100 reactions), is however of more concern. These ratios typically originate from older evaluations, which are generally of reasonable quality, except in the pre-equilibrium range, where an approximative treatment was applied. Since (n,γ) cross sections around 14 MeV are not practically very important, the data have been retained for the current version. The small number of reactions with very small values of C/S are all for very low mass targets for which the systematics are not applicable.

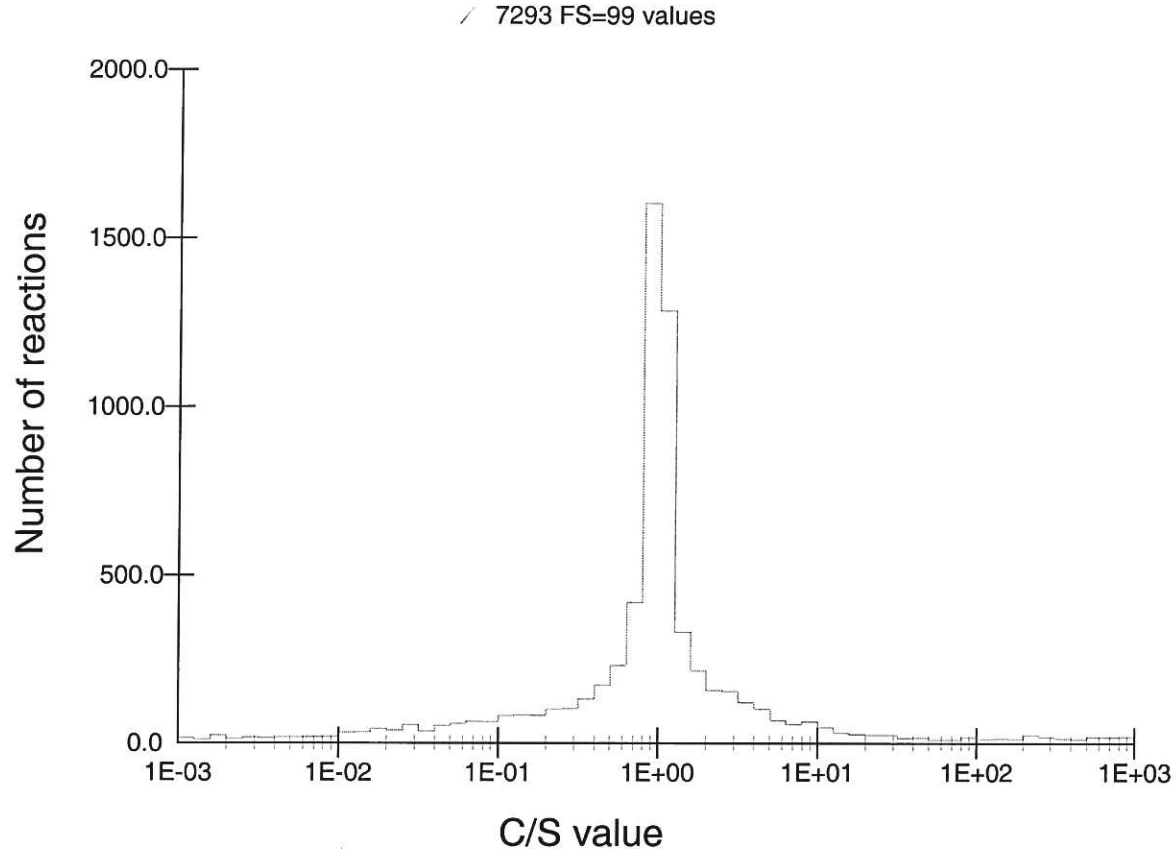

Figure 17. C/S distribution at 14.5 MeV for all reactions in EAF-2001.

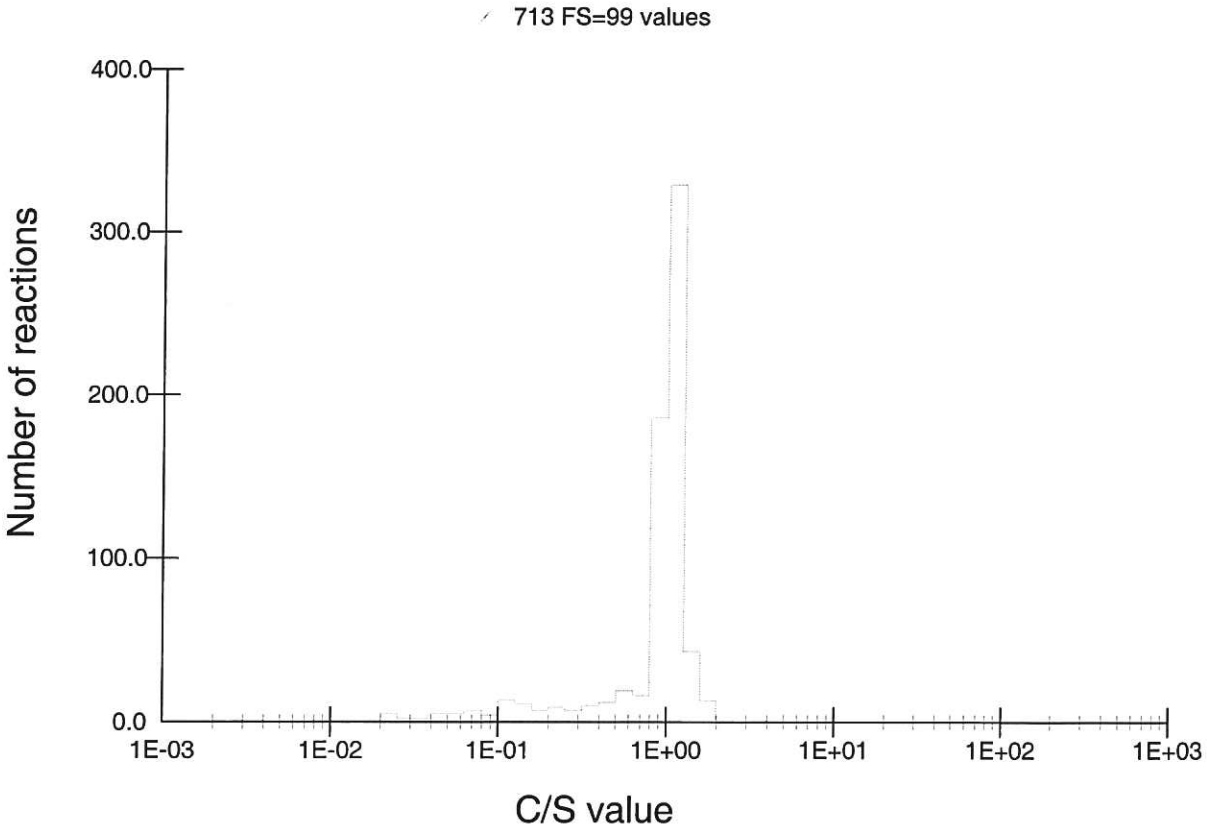

Figure 18. C/S distribution at 14.5 MeV for (n,2n) in EAF-2001.

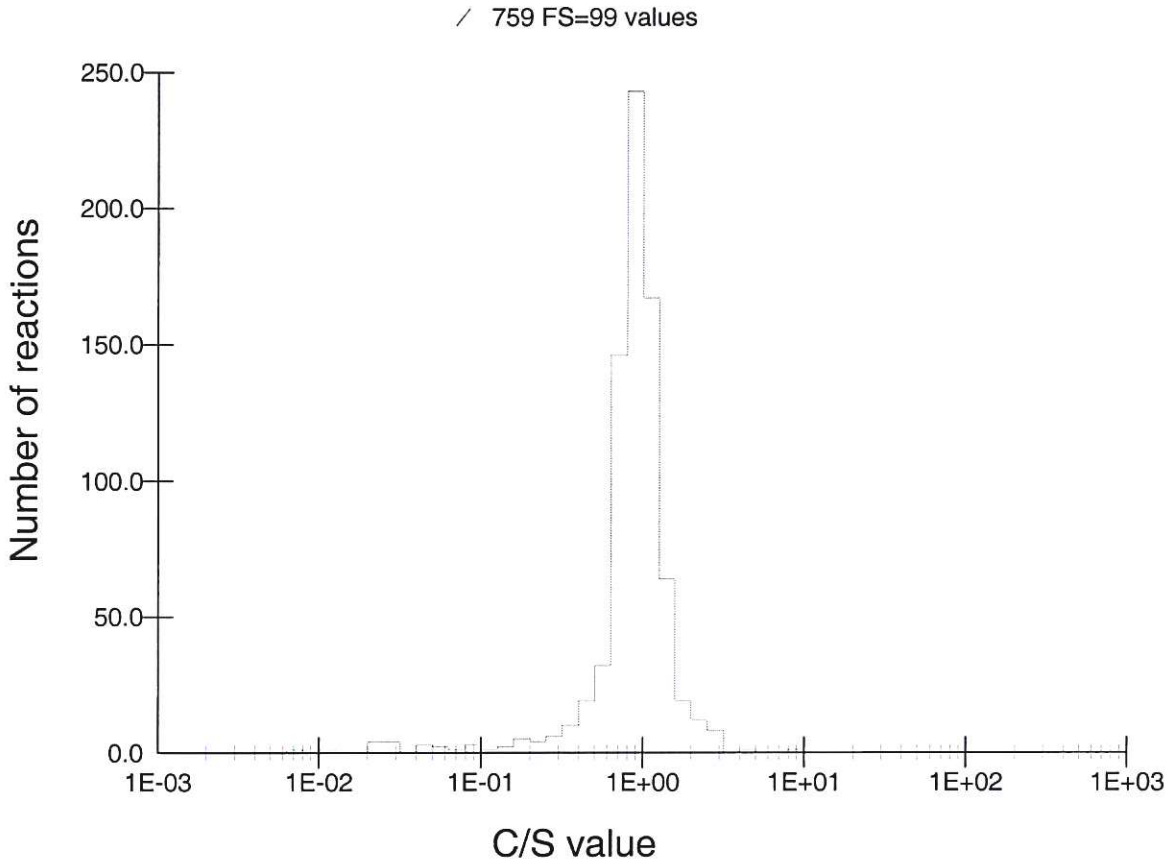

Figure 19. C/S distribution at 14.5 MeV for (n,α) in EAF-2001.

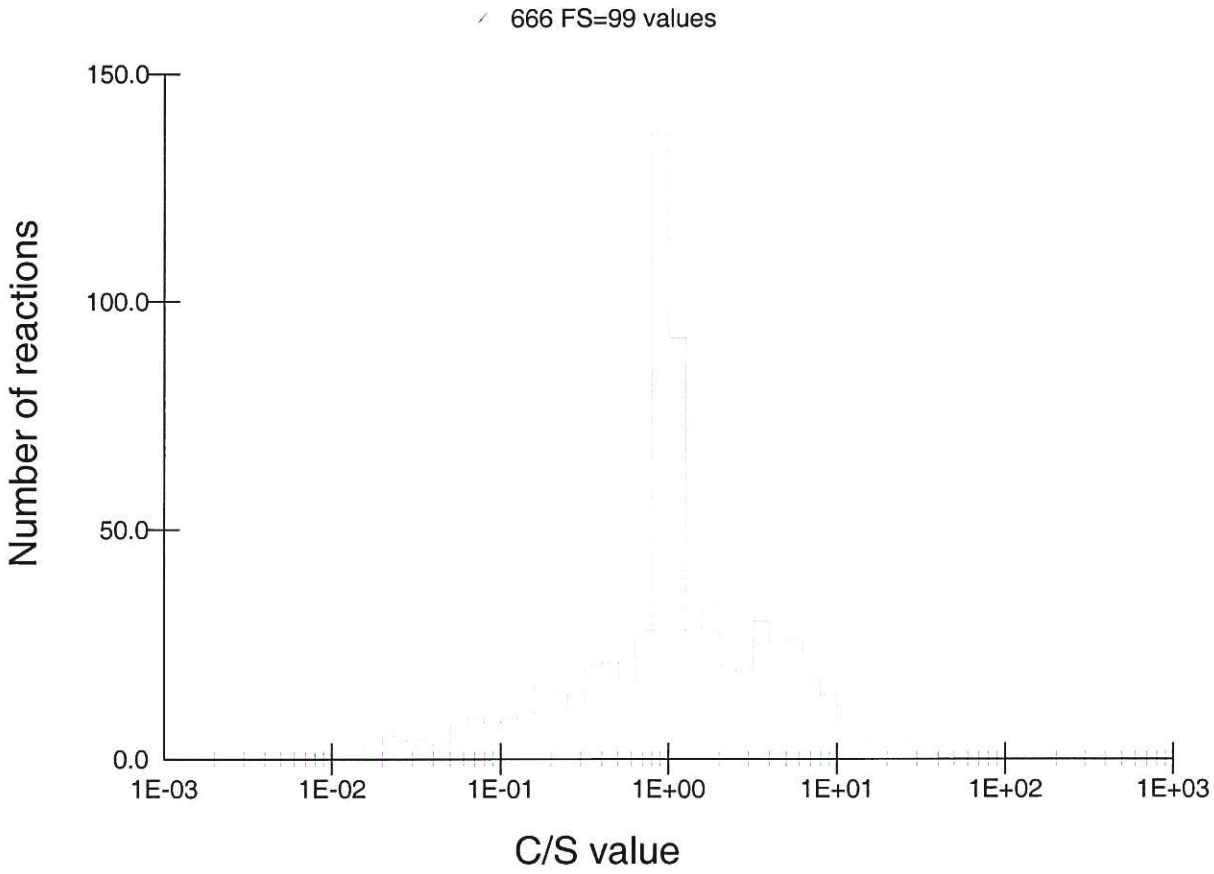

Figure 20. C/S distribution at 14.5 MeV for (n,d) in EAF-2001.

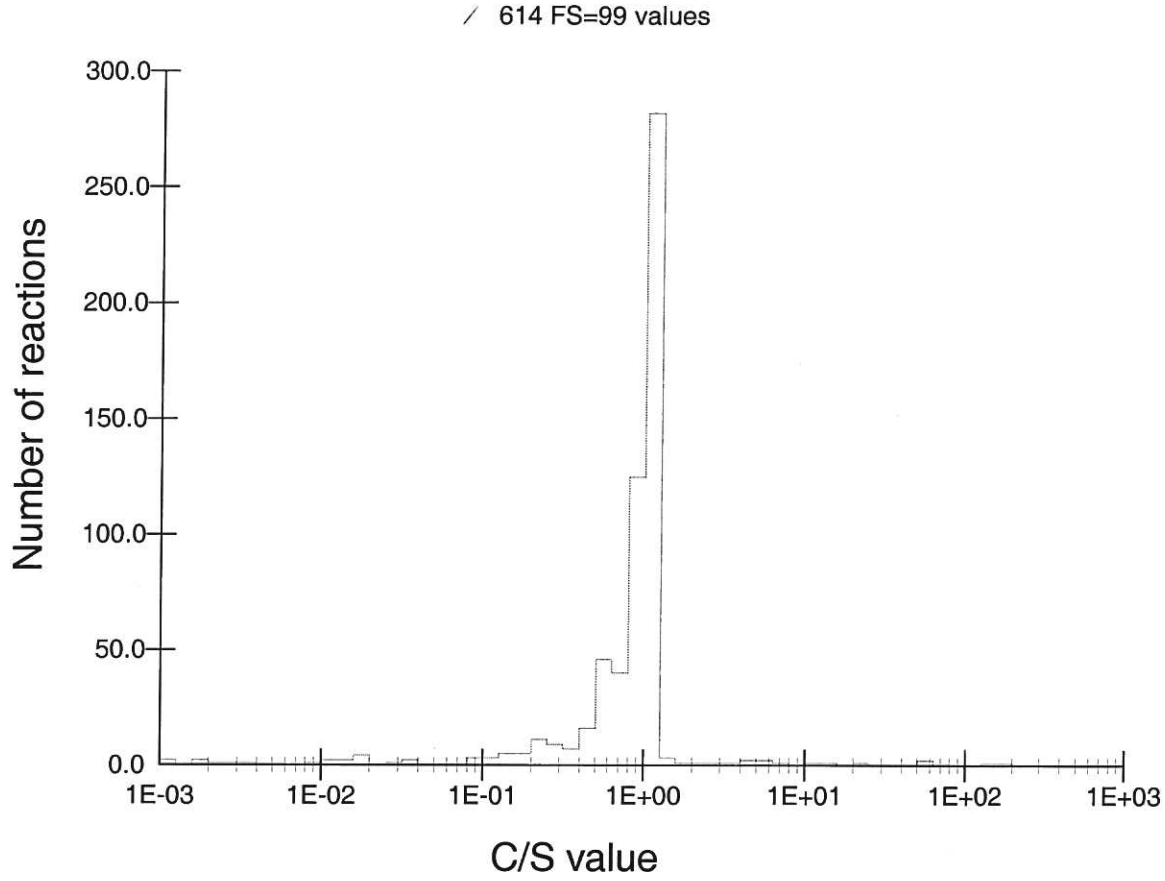

Figure 21. C/S distribution at 14.5 MeV for (n,h) in EAF-2001.

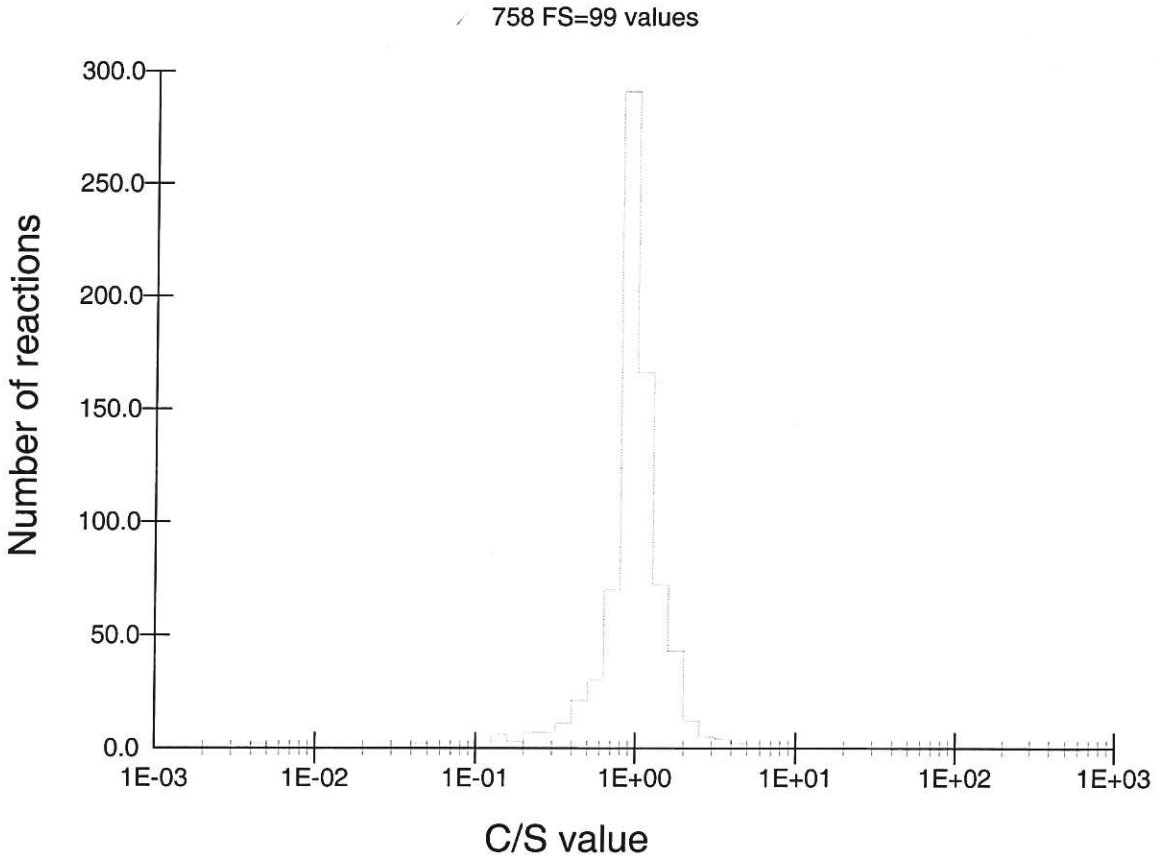

Figure 22. C/S distribution at 14.5 MeV for (n,p) in EAF-2001.

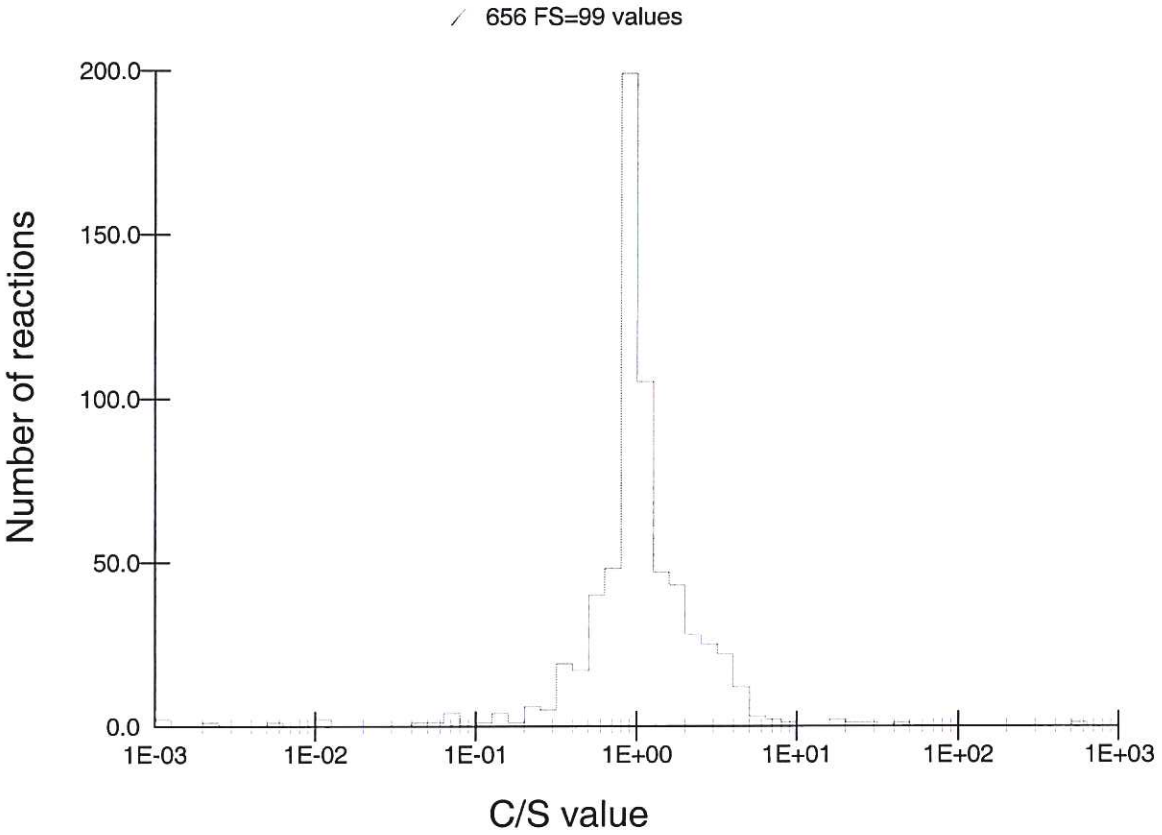

Figure 23. C/S distribution at 14.5 MeV for (n,t) in EAF-2001.

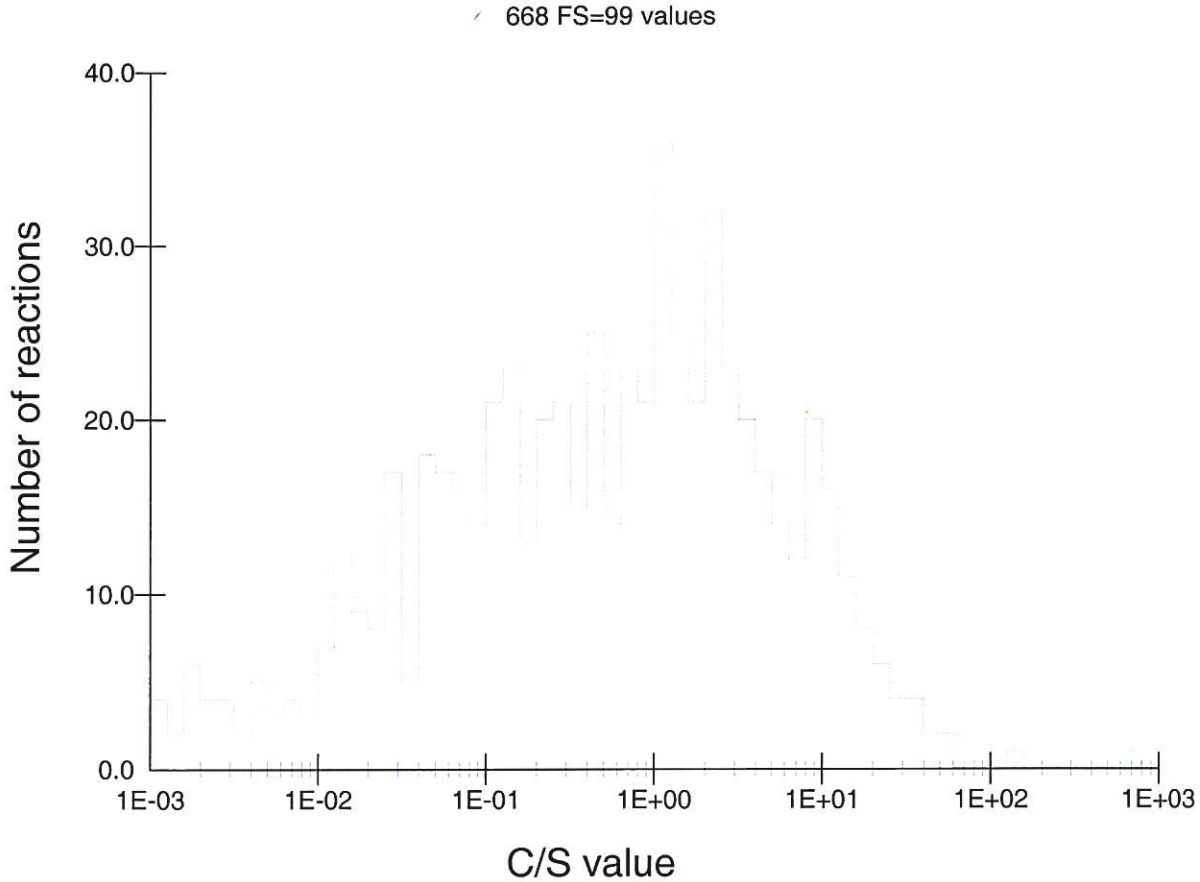

Figure 24. C/S distribution at 14.5 MeV for (n,n'α) in EAF-2001.

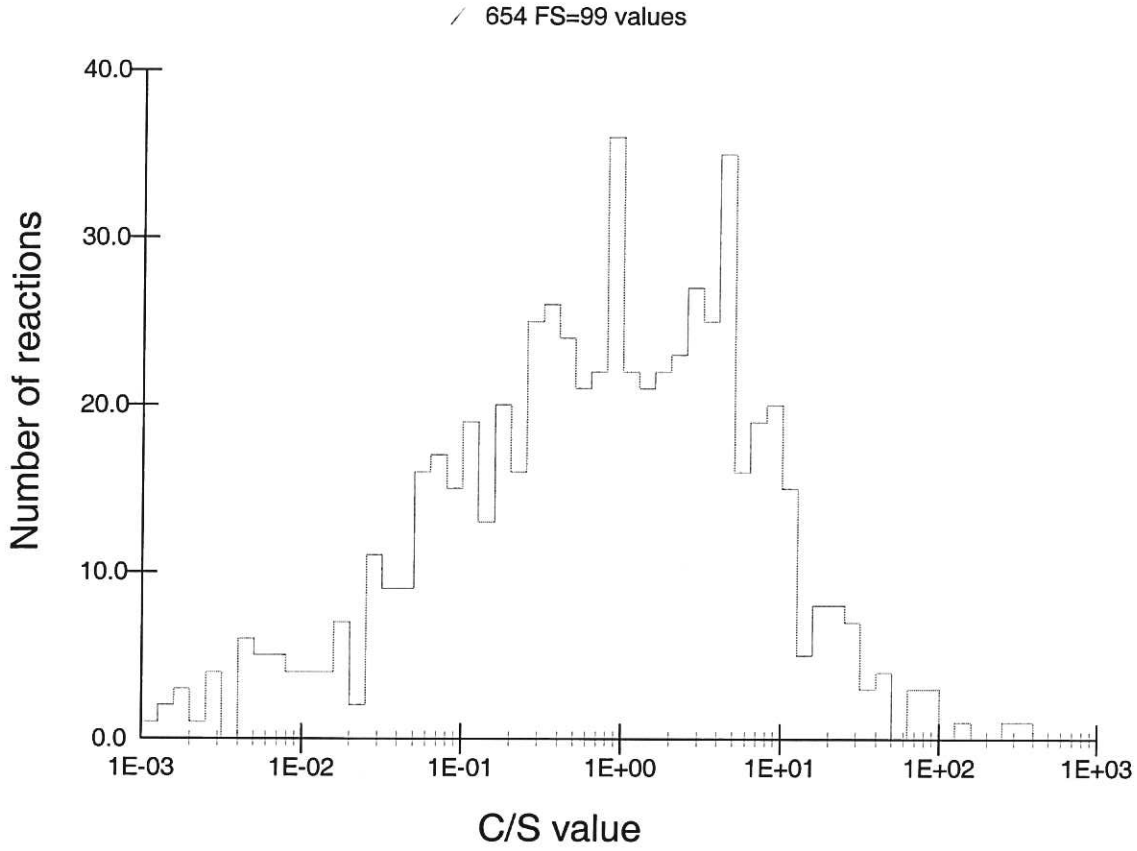

Figure 25. C/S distribution at 14.5 MeV for (n,n′p) in EAF-2001

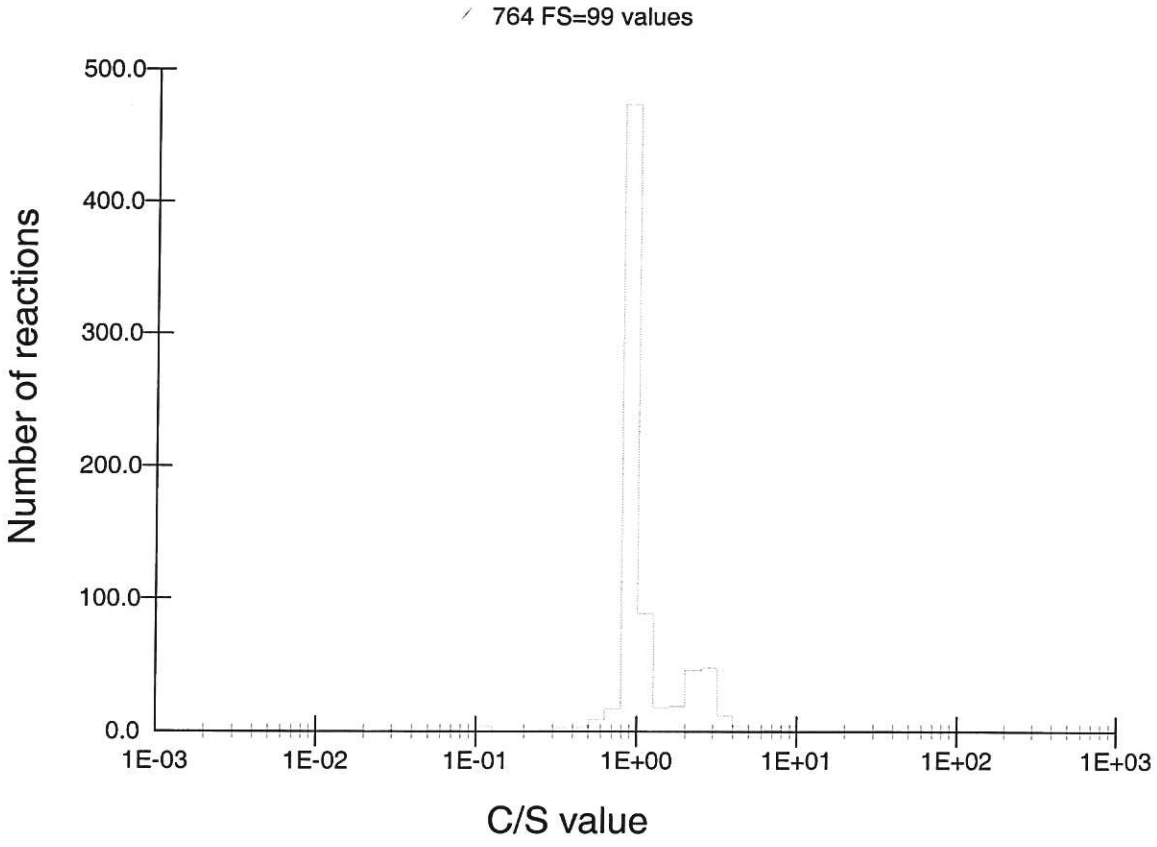

Figure 26. C/S distribution at 14.5 MeV for (n,γ) in EAF-2001.

EAF-2001 uncertainty file

A complete uncertainty file is generated by SAFEPAQ-II for the EAF-2001 cross section data library. The file is in the ENDF-6 MF = 33 format, and contains uncertainty data in a one-group format for threshold reactions from the threshold to 20 MeV. A three group format is adopted for the (n,γ) and (n,f) reactions: from 10^{-5} eV to E_V (the end of the $1/v$ region), E_V to E_H (the end of the resonance region) and E_H to 20 MeV. The uncertainty values adopted correspond to the error factor f:

$$f = 1 + \Delta$$

where Δ is the relative error (Δ^2 is actually stored in the file) in the cross section σ. In this case the best estimate of the cross section uncertainty is:

$$\sigma/f < \sigma < \sigma f$$

The emphasis for EAF-2001 uncertainties has been to include as much as possible of the experimental information. The ultimate goal is that in the future, all reactions, (about 1800) present in either EXFOR or the Parameter tables will be provided with uncertainty factors derived from experimental information. For threshold reactions experimental variance information at 14 MeV is available for 867 reactions. These uncertainties have been estimated from the data scatter around adopted excitation curve in EXFOR plots or from the now growing data base of experimental validation [100 - 115]. This 14 MeV experimental variance is used for the entire energy range of the excitation function, and because no information on uncertainties at other energies has been used, an uncertainty value of $\Delta\sigma = 3\Delta\sigma_{exp}$ has been adopted. This represent a 99.9% confidence limit. For (n,γ) and (n,f) reactions, thermal cross section and resonance integral information are used for the first two energy ranges. For the smooth statistical range the uncertainty factor is usually estimated from the scatter of EXFOR data around the evaluated curve.

In the numerous cases where no experimental values are available, the uncertainty is extracted from systematics, results of graphical information or estimates (see Table 2). Depending on the reaction type, data origin and energy range the uncertainty value may vary from less than one percent to a factor of five in exceptional cases. The bulk of the uncertainties however, range from a few percent to a factor of two.

Another important aspect of the uncertainty treatment occurs when the cross section is split. In general for uncertainties of cross sections to ground and isomeric states an uncertainty factor of the branching ration (f_b) of 1.3 has been adopted when the branching is derived from systematics.

By definition $\sigma_m = b\sigma$ and $\sigma_g = (1-b)\sigma$. Thus the uncertainty in σ_m is given by:

$$\left(\frac{\Delta\sigma_m}{\sigma_m}\right)^2 = \left(\frac{\Delta b}{b}\right)^2 + \left(\frac{\Delta\sigma}{\sigma}\right)^2$$

and $\Delta\sigma/\sigma = f - 1$ and $\Delta b/b = f_b - 1$. Thus:

$$f_m = f_g = 1 + \sqrt{f_b^2 + f^2 - 2(f + f_b - 1)}$$

If experimental values of partial cross sections are known their uncertainties are adopted, although this is rare. Such a method of uncertainty propagation to the partial cross sections is certainly pessimistic although if no experimental data exist for the branching ratio their generation using systematics is not without error and an uncertainty of 30% is considered as sound pending further investigation.

An example of the EAF uncertainty file format is given in Appendix 1. Further details of the uncertainties and their use in FISPACT are presented in reference 1.

EAF data formats

Pointwise data formats

The format of the EAF-2001 file is essentially that of the MF = 3 file of ENDF-5 format with the following deviations (the resulting format is usually referred to as the EAF format):

- Two comment lines have been added at an earlier stage, stating the origin of data and the SAFEPAQ-II modifications.
- The material number MAT consists of Z and the two last digits of A. To describe isomeric targets A has been increased by 50 or 70 (m or n, respectively). Consequently, the order of the cross sections (according to increasing MAT numbers) is not always in accordance with increasing Z and A. This applies only to the pointwise format data, not to the multigroup constant library, for which another MAT number with more digits is used.

- The identifiers LIS and LFS are used to indicate the (isomeric) states of the target and final nucleus, respectively. Here we have adopted the convention that LFS = 99 means total production cross section; LFS = 0, 1, or 2 means production of ground state, first and second isomeric state, respectively.
- The reaction nomenclature is as defined by ENDF, except that reaction numbers leading to isomeric states have been increased by 300 or 600 (for m and n, respectively). The cross sections for one material number are ordered according to increasing MT numbers, except that cross sections leading to isomeric states follow immediately after the cross section leading to the ground state.

The composition of the comment lines has been fully described in an earlier section. An example of the EAF pointwise file format is given in Appendix 2.

Groupwise data formats

SAFEPAQ-II calculates the multigroup file using a new procedure, this is fully described in reference 2. The format of the multigroup library, GXS_EAF, is the LIBOUT format of the code FOUR ACES (ENEA Bologna), again with two additional comment lines (modification data is shown on the first, the second is blank) for each reaction. For reaction numbers the ENDF-reaction number MT multiplied by 10 has been adopted, with the convention that for the excitation of each isomeric state the reaction number is increased by one. The material numbers of EAF_GXS consist of Z, A and an identifier to indicate ground or isomeric target (MAT = Z x 10000 + A x 10 + LIS). The order of the cross sections on the EAF_GXS file is in accordance with increasing Z, A, LIS, LFS and MT.

The multigroup file is produced in one of five group-structures: that of GAM-2 (100 groups), VITAMIN-J (175 groups), WIMS (69 groups), XMAS (172 groups) and TRIPOLI (315 groups) with appropriate flux-weighting spectra. However, if required the group structure could be changed into any energy group structure or weighting function with a small amount of effort.

The accuracy of a set of multigroup constants is determined by the group structure and the weight function. This is particularly true when either the group structure is coarse (*e,g.* VITAMIN-J in the thermal range) or when the flux varies strongly between different regions of the device. Historically all of the weighting functions included a fission spectrum but that is not appropriate when the device is a fusion plant. Similarly having a fusion

peak in the weight function used for a fission plant is not correct. Three distinct weight functions have been used to process the groupwise files. They are denoted as:

- FLA or FLT: a flat or constant weight function (not shown).
- FIS : this weight function combines a thermal Maxwellian at low energies, a $1/E$ function at intermediate energies, and a fission spectrum (T = 1.3539 MeV) with a fast dropping tail at higher energies shown in Figure 27.
- FUS: this weight function combines a thermal Maxwellian at low energies, a $1/E$ function at intermediate energies, and a velocity exponential fusion peak spectrum with a peak at 14.07 MeV shown in Figure 28.

An example of the EAF groupwise file format is given in Appendix 3.

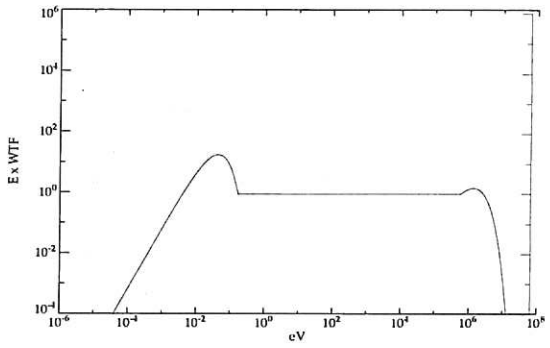

Figure 27. EAF-2001 micro-flux weighting function for fission.

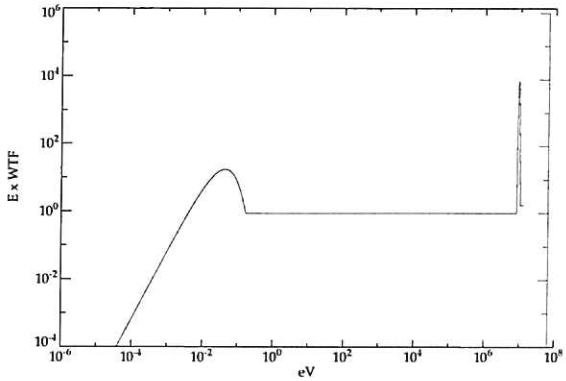

Figure 28. EAF-2001 micro-flux weighting function for fusion.

Conclusions

The neutron-induced cross section data included in comprehensive activation files such as EAF-2001 come from sources having varying degrees of quality. The processing code SAFEPAQ-II enables all the necessary modifications to be performed in a well defined and quality assured manner. This leads to the creation of an activation file that can claim a much higher degree of quality than the original sources. The validation of the processed data, in various energy ranges, allows the correctness of the data treatments to be certified at the processing stage.

However, it is important to note that although the file is probably as complete as required for magnetic fusion applications, the experimental database that allows internal validation by C/E analysis is far from complete and contains many deficiencies. Although systematic comparisons can be made at high energies, the derived uncertainty margins are higher and rely more on estimation than on an experimental comparison. This introduces higher calculational uncertainties and so forces wider safety margins for applications that rely on 14 MeV data. A greater range of experimental measurements is therefore urgently required.

In EAF-2001 results of integral experiments have been used to adjust data. Validation of activation code predictions, and thereby of cross section and decay data, has been performed by means of direct comparison with measurements of sample structural material under fusion-relevant neutron spectra. Integral experiments are a rich source of information with which a wide range of validation and comparison exercises can be made in the activation data field. The broad trends of the time dependent values of the calculated-to-experimental ratios represent the best estimates of the uncertainties that should be applied to predictions made with activation codes.

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Disclaimer

Neither the authors nor UKAEA accept responsibility for consequences arising from any errors either in the present documentation or in the EAF libraries.

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Feedback on the use of EAF is welcomed. Please contact RA Forrest with comments or in case of problems.

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Appendix 1: EAF uncertainty format

An extract from the uncertainty file is given below for ^{48}Ti to illustrate the format.

```
TI- 48N,2N                                                              224833 16
 2.20480E+4 4.7536E+01          0          0          0          1224833 16
 0.0000E+00 0.0000E+00          0         16          0          1224833 16
 0.0000E+00 0.0000E+00          0          1          6          3224833 16
 1.0000E-05 0.0000E+00 1.1875E+07 4.0000E-04 2.0000E+07 0.0000E+00224833 16
                                                                 224833  0
TI- 48N,NA                                                              224833 22
 2.20480E+4 4.7536E+01          0          0          0          1224833 22
 0.0000E+00 0.0000E+00          0         22          0          1224833 22
 0.0000E+00 0.0000E+00          0          1          6          3224833 22
 1.0000E-05 0.0000E+00 9.6386E+06 4.0000E+00 2.0000E+07 0.0000E+00224833 22
                                                                 224833  0
TI- 48N,NP                                                              224833 28
 2.20480E+4 4.7536E+01          0          0          0          1224833 28
 0.0000E+00 0.0000E+00          0         28          0          1224833 28
 0.0000E+00 0.0000E+00          0          1          6          3224833 28
 1.0000E-05 0.0000E+00 1.1683E+07 1.0000E+00 2.0000E+07 0.0000E+00224833 28
                                                                 224833  0
TI- 48N,G                                                               224833102
 2.20480E+4 4.7536E+01          0          0          0          1224833102
 0.0000E+00 0.0000E+00          0        102          0          1224833102
 0.0000E+00 0.0000E+00          0          1          8          4224833102
 1.0000E-05 1.1696E-01 1.0000E+03 2.7889E-02 1.0000E+05 1.0000E+00224833102
 2.0000E+07 0.0000E+00                                           224833102
                                                                 224833  0
TI- 48N,P                                                               224833103
 2.20480E+4 4.7536E+01          0          0          0          1224833103
 0.0000E+00 0.0000E+00          0        103          0          1224833103
 0.0000E+00 0.0000E+00          0          1          6          3224833103
 1.0000E-05 0.0000E+00 3.2793E+06 2.5000E-03 2.0000E+07 0.0000E+00224833103
                                                                 224833  0
TI- 48N,D                                                               224833104
 2.20480E+4 4.7536E+01          0          0          0          1224833104
 0.0000E+00 0.0000E+00          0        104          0          1224833104
 0.0000E+00 0.0000E+00          0          1          6          3224833104
 1.0000E-05 0.0000E+00 9.4122E+06 1.8490E-01 2.0000E+07 0.0000E+00224833104
                                                                 224833  0
TI- 48N,T                                                               224833105
 2.20480E+4 4.7536E+01          0          0          0          1224833105
 0.0000E+00 0.0000E+00          0        105          0          1224833105
 0.0000E+00 0.0000E+00          0          1          6          3224833105
 1.0000E-05 0.0000E+00 1.3896E+07 7.2000E-01 2.0000E+07 0.0000E+00224833105
                                                                 224833  0
TI- 48N,T*                                                              224833405
 2.20480E+4 4.7536E+01          0          0          0          1224833405
 0.0000E+00 0.0000E+00          0        405          0          1224833405
 0.0000E+00 0.0000E+00          0          1          6          3224833405
 1.0000E-05 0.0000E+00 1.4044E+07 7.2000E-01 2.0000E+07 0.0000E+00224833405
                                                                 224833  0
TI- 48N,H                                                               224833106
 2.20480E+4 4.7536E+01          0          0          0          1224833106
 0.0000E+00 0.0000E+00          0        106          0          1224833106
 0.0000E+00 0.0000E+00          0          1          6          3224833106
 1.0000E-05 0.0000E+00 1.2465E+07 8.1000E-01 2.0000E+07 0.0000E+00224833106
                                                                 224833  0
TI- 48N,A                                                               224833107
 2.20480E+4 4.7536E+01          0          0          0          1224833107
 0.0000E+00 0.0000E+00          0        107          0          1224833107
 0.0000E+00 0.0000E+00          0          1          6          3224833107
 1.0000E-05 0.0000E+00 2.0741E+06 1.0000E-02 2.0000E+07 0.0000E+00224833107
                                                                 224833  0
TI- 48N,2P                                                              224833111
 2.20480E+4 4.7536E+01          0          0          0          1224833111
 0.0000E+00 0.0000E+00          0        111          0          1224833111
 0.0000E+00 0.0000E+00          0          1          6          3224833111
 1.0000E-05 0.0000E+00 1.2926E+07 4.0000E+00 2.0000E+07 0.0000E+00224833111
                                                                 224833  0
```