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EUROPEAN ACTIVATION FILE FOR FUSION

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Abstract: This paper describes the work performed to revise and extend the European Activation File (EAF). The extensions, revisions and improvements made in the first two versions of the file (EAF-1, EAF-2) are discussed as well as the work which is planned for EAF-3. The EAF-2 file contains cross-sections for all stable and unstable nuclides with half-lifes exceeding 0.5 day. Cross-sections leading to isomeric states are given separately and those isomeric states with $T_{1/2}$ > 0.5 d are included as targets. The EAF-2 version contains about 11000 reactions on 667 targets. The EAF-2 data file will be further extended and improved and will be supplied with uncertainty information.

(Neutron activation cross sections, incident energies up to 20 MeV).

Introduction

The aim of this work was to provide a complete system for a European activation data library (EAF) which together with the inventory code FISPACT [1] and its associated data libraries will be used for activation and transmutation calculations in fusion reactor technology problems. The importance of studying low activation materials to ensure that future reactors ner as safe as possible and environmentally benign has accelerated the need for a complete and yet high-quality activation file. Another emphesis has been on improvement of the (n,γ) data in view of the importance of the low-energy component in neutron spectra in fusion reactors. The strategy and goals for the creation of activation files in the framework of the European Technology Programme are as follows:
1. Address the completeness of the library using the well tested mass-production means of the EAF files such as simple model codes and systematics. Extend further the library with actinide targets (EAF-3).
2. Provide the library with a simple but complete uncertainty file which will enable routine uncertainty estimates and sensitivity studies to be carried out (EAF-3).
3. Based on sensitivity studies, the feedback of information from users and benchmark testing, will improve the quality of selected important reaction cross sections with full evaluations or data adopted from other libraries (e.g. JEF-2, EFF-2, ENDF/B-6, JENDL-3). This will be a continuing activity for all future versions of EAF.
As a starter file for this exercise the last version from the series of REAC-ECN files [2,3] - REAC-ECN-5 - has been used, together with some information from the UKACT1 file of AEA Harwell. The basis of the revision into EAF-1 was an update of renormalizations to 14.5 Mev experimental data or to data from systematics. In particular data for the neutron emission channels (n,n'), (n,2n) and (n,3n) have been improved. Another aspect was to extend the library so as to achieve a library which contains all stable and unstable targes with half-lifes longer than 0.5 day. Cross sections leading to isomeric states are treated separately and further those isomeric states with half-lifes longer than 0.5 day are included as targets. To ensure that gas production (e.g. ^{3}H and ^{4}He) is calculated correctly, different reactions leading to the same daughter nuclide are given separately. The present version of EAF-2 contains now about 11000 reactions on 667 targets. The major improvement, however, was a complete revision and re-evaluation of radiative neutron capture cross sections.
The point wise file EAF-1 was released in January 1990. The present version EAF-2 which was released in May 1991 is described in this paper and in more detail in the laboratory report [5]. Both data files have been processed into the multigroup library GEAF with either 100- (GAM-II) or 175 group (VITAMIN-J) structures.

Evaluation methods

Techniques which have been applied in the evaluation of the EAF files have been documented in refs. [2-4]. They consisted mainly of two codes to calculate excitation funtions (THRES and FISPRO-ECN), the application of cross-section systematics of Forrest [6], Vonach [7] and Kopecky [2] and the use of Kopecky et al. systematics of isomer ratios [3,8]. Recent extensions and improvements are discussed below.

1. Nuclear models for excitation functions

In general we have still adopted the code THRES [9] as a main source for calculation of excitation curves (except for radiative capture) if no other evaluation was available for the target nuclide. Because of severe shortcomings of THRES, we have applied several corrections to the calculated data, based on comparisons with "horizontal" evaluations and/or experimental data.
The neutron emission cross sections as modelled in THRES have been improved in the following way:
(i) The (n,n'γ) cross sections to metastable states were derived in two steps. First the branching ratio systematics for one-step reactions [8] was applied to the THRES results of the total inelastic cross section. Then a constant component was added, modelling in a

crude way the pre-equilibrium part, to reach the value of the systematics of Vonsch [7] at 14.5 MeV.
(ii) In order to correct for (n,3n) cross sections, set too high by THRES, all (n,3n) cross sections were decreased by 20% so that neutron emission cross sections were in agreement with systematics. This factor has been derived from available experimental information and seems to be a rather reasonable approximation [5].
(iii) For target nuclides with the (n,3n) threshold below 14 MeV, and thus the (n,2n) excitation function around 14 MeV possessing a steep fall, no renormaliza- tions have been applied.
The effective threshold energies for all reactions leading to isomeric states have been implemented. Cross sections for isomeric targets are so far assumed to be identical to those for the ground-state.

2. Evaluation of radiative capture data

Completeness and quality of the radiative capture data were the main objectives of the recent version of the EAF. The (n,γ) reaction is important at relatively low energies and therefore the thermal and resonance ranges have been fully reconsidered.
In the re-evaluation of the radiative cross sections the targets were categori- zed in three groups:
1. complete evaluation available, including resolved resonance parameters, in existing general purpose files;
2. no evaluation is available but experimental information exists;
3. no experimental information exists.

In the first group all existing evaluations (JEF-1, JENDL-3, ENDF/B-6) have been adopted to replace the old data. These evaluations are tested against the experimental data and include a resolved resonance region. Thus they belong to the category with the highest accuracy, however, some do not have a proper direct/semidirect component. This omission results in a 14.5 MeV value well below the systematic value. For the re maining targets (groups 2 and 3) new calculations have been performed with two ECN codes, FISGIN and MASGAM. In the case of group 2 a special evaluation in the resolved and thermal energy range was made with the help of the code SIGECN and included in the file. The contents of the EAF-2 (n,γ) subfile is summarized in Table 1.

Table 1. List of sources for (n,γ) data in EAF-2

Data source	Number of targets
JEF-1	246
ENDF/B-5,6	18
JENDL-3	32
Other evaluations	5
FISGIN	6
MASGAM + SIG-ECN	57
MASGAM	303
Total	667

2.1 Applied nuclear models for calculation of (n,γ) excitation functions

FISGIN [10] is an improved version of the code FISPRO (originating from ENEA Bologna), a Hauser-Feshbach statistical- model code with a direct-semidirect component of Lane-Lynn-Brown. It also allows the calculation of smooth backround cross sections due to missed resonances. Available information on the resolved resonance region is generated with the code SIG-ECN and included in a point-wise format. The calculation is checked against experimental data and these evaluations can be considered to reach the same quality as the first category. This approach has been applied for reactions from group 2 having the status of an important reaction.
MASGAM [11] is a simplified version of FISGIN provided with 1/v-, statistical- and pre-equilibrium components. Recognizing difficulties of the direct-semidirect approach to reproduce the experimental data of excitation curves above 6 MeV, the systematics of Ref.[12] was implemented instead. This rather empirical systematics, despite several simple assumptions, fits the experimental data reasonably well. The final formula reads as

$$\sigma_{n\gamma}(DSD) = C \int_{0}^{S_n+E_n} \frac{E_R^4 (E_\gamma^2 - E_R^2)^2 + E_\gamma^2 \Gamma^2}{E_n^3 [1 + 0.035A(1 + S_n/E_n)^3]} dE,$$

where E_γ, E_n and E_R are gamma-ray-, neutron and the giant-resonance energies, Γ is the spreading width, S_n is the neutron threshold (all in MeV) and C is a constant independent of energy. Contrary to the original approach, where this constant was globaly adjusted to experimental data to reproduce absolute cross-section values, we applied the systematics at 14.5 MeV [2] instead. The input of data to MASGAM is fully automated. It uses a minimal input information such as Z, A and the level scheme of the target nuclide. It assumes only E1 radiation and all the other relevant parameters, such as the optical-model parameters, the level density- and the E1-giant resonance parameters are derived from global systematics. An example of the calculation for a target nuclide with A=150 is given in Fig. 1. This procedure is discussed in detail in Ref. [11]. The smooth statistical region is coupled to a 1/v-component at the energy $E_\lambda = 0.5\ D_0$. The calculated values can be checked and renormalized at three neutron energies, namely 0.0253 eV, 30 keV and 14.5 MeV. A comparison of MASGAM results (before renormalization) for the ^{143}Nd target with the JEF-1 evaluation is displayed in Fig. 2.
If experimental information on the resolved resonance region exists [13], the code SIG-ECN has been used to generate a point-wise file based on the resonance parameters. Merging these data with the MASGAM smooth results have been carried out within the processing code SYMPAL. The energy E_M, at which both data are joint, is determined in the following way. Both files have been processed into the Vitamin-J group structure and were graphically compared to identify the energy at which it seems resonances start missing, as compared to the calculated smooth statistical part. The group boundary

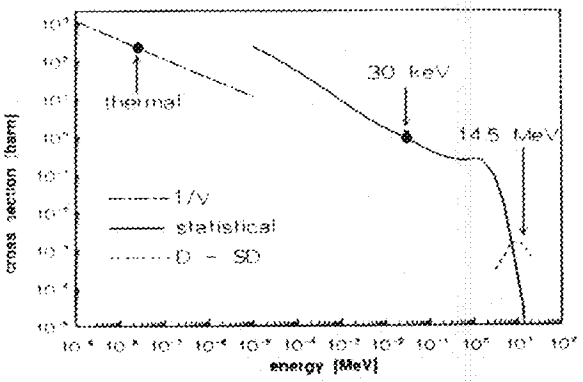


Fig.1. The (n,γ) excitation curve as calculated with the code MASGAM for an even target with A ≈ 150. Three components are dispayed separately with their normalization points.

prior to this energy has been chosen as E_n. This rather simple and quick procedure has been tested against some existing earlier evaluations and turned out to be reasonably good. These data are denoted in Table 1 as MASGAM + SIG-ECN.

2.2 Applied renormalizations

If experimental information on cross sections is available, it is used to renormalize the calculated component of the excitation curve separately. The 1/v-component is adjusted to agree at 0.0253 eV with the thermal cross-section value [13] and the smooth statistical component is adjusted at 30 keV, where a large amount of cross section data exist from astrophysics studies [14]. The compilation of Wagner and Warhanek [15] was used for the direct/semidirect (DSD) component at 14.5 MeV. The calculated excitation curve, renormalized in this way, has a large uncertainty mainly in the resonance region, if the resolved resonance data are unavailable (see table 2 for details).
In order to provide additional renormalization systematics, if no experimental information is available, e.g. for radioactive targets, an attempt has been made to develope systematics both for thermal data and for the 30 keV data. The prediction of thermal cross sections is almost impossible, due to the fact that only a limited number of resonances determine these values and thus no statistical assumptions can be applied. However, in spite of the expected very large uncertainty in these "predictions" some attempt is made to account for at least the global trend.
Starting from the expression for the average capture cross section, after several simplifications, the parameterized formula

$$\sigma_{n\gamma} \approx C\,(aU)^X$$

can be used to fit the constants C and X to the measured data. U is the effective excitation energy, defined as $U = S_n$ - pairing energy, and a is the level density parameter.
First a least-squares fit was applied to the thermal cross-section data (compliled in [13]), with a and U values derived from systematics applied in the code MASGAM. The results are displayed in Table 2 and fig.3 and show that the pairing correction smoothed to some extent the

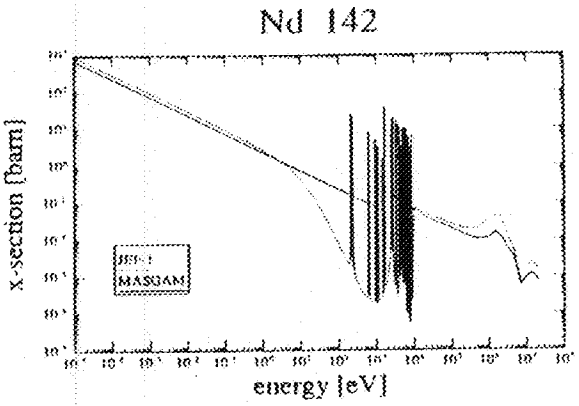


Fig.2. A comparison of MASCAM and JEF-1 data for the ^{141}Nd(n,γ) reaction before renormalization at 0.0253 eV and 30 keV. Mind the D-SD component in NEF-1, which is too large compared to the systematics.

raw data. However, as expected the scatter of the data around the fitted curve remains large with deviations of a factor f≈50 or more.
A similar procedure has been applied to the 30 keV data (compiled in [14]) separately for odd- and even-Z targets. The results are displayed in figs. 4 and 5 and in Table 2 and show an acceptable scatter of data arround the fitted curves with deviations of a factor 1.5 - 2.0.

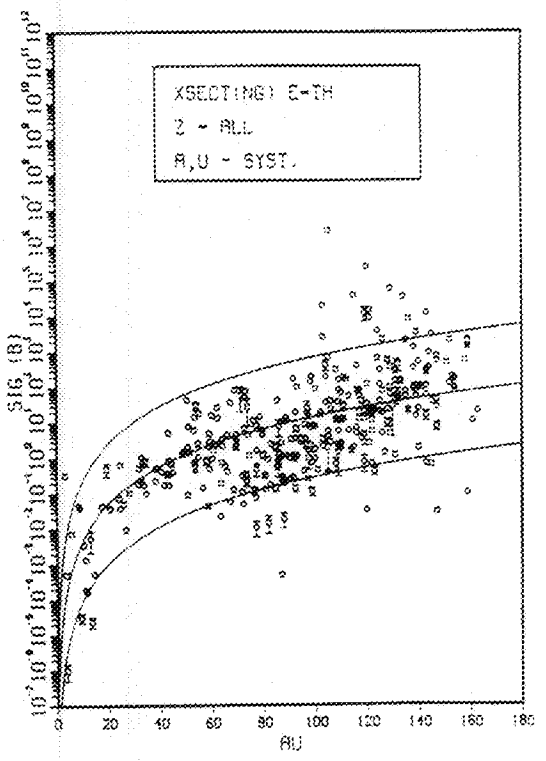
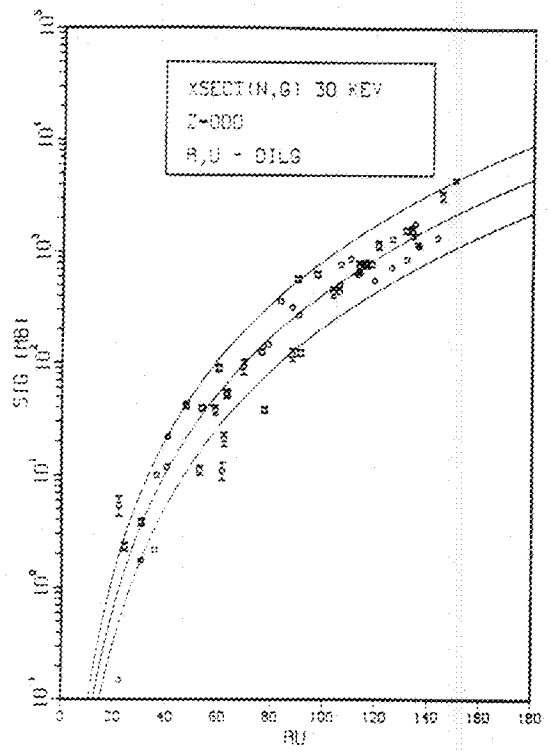


Fig.3. Thermal capture cross sections (taken from ref. [13]) plotted against aU together with the fitted curve. The uncertainty band with f=50 is indicated.



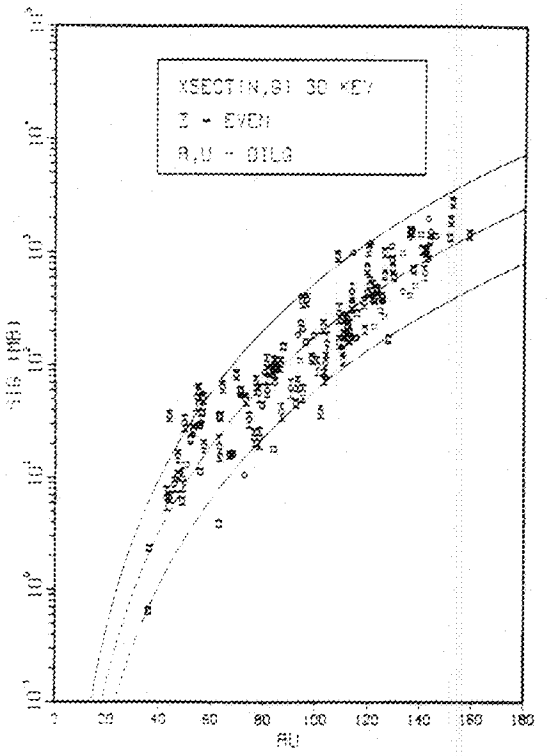


Fig.4 and 5. Average capture cross sections at 30 keV (adopted from [14]) or odd-(even)-Z targets, respectively, plotted against AU together with their uncertainties of f=1.5 and f=2, respectively.

Table 2. Derived systematics to fit the MASGAM calculations

$\sigma_{n\gamma}(E_n)$	LSQ-fit
$\sigma_{n\gamma}$(th)	$1.5E\text{-}6\ (aU)^{3.5}$
$\sigma_{n\gamma}$(30 keV)	
Odd-Z	$3.346E\text{-}6\ (aU)^{4.025}$
Even-Z	$2.461E\text{-}7\ (aU)^{4.41}$
$\sigma_{n\gamma}$(14.5 MeV)	$1.18\text{-}1.13\ e^{-0.01338A}$

The full procedure of MASGAM calulations and renormalizations has been tested against several JEF-1 evaluations across the entire mass range and showed a very good egreement, considering all the approximations applied (for results see [11]). The adopted uncertainties, both due to the applied model and the renormalizations, are given in table 3.

Table 3. The estimated uncertainties of the MASGAM calculations

MASGAM renormalization	Energy component		
	1/v	Stat.	D-SD
experiment	$\Delta\sigma_{n\gamma}$	1.5[a,b]	1.5[b]
systematics	100	3.0[b]	1.5[b]

[a] Except the energy region between $D_0/2$ and several tens of D_0, where the absent resonance cross sections introduce a large uncertainty.

[b] Includes also the guessed uncertainty of the statistical and DSD model in the energy ranges considered.

3. Renormalizations at 14.5 MeV to systematics

Several new systematics have been derived in recent few years. They estimate mainly the cross-section values at 14.5 MeV. However, some derive also the shape of the excitation curve. The list concerning only the 14.5 MeV values can be summarized as follows: (n,2n) [15,16]; (n,p) [15,17,18]; (n,d+n,np) [15,19]; (n,α) [15].
The references on the systematics of the excitation curves are: (n,charged particle) [20]; (n,np),(n,nα) [21] and (n,γ) [22].
These systematics have been compared with the set of those adopted earlier during the development of REAC-ECN files, based essentially on three authors: Forrest [6], Vonach [7] and Kopecky [2]. The comparison was done only graphically, the systematics against each other together with the available experimental data. We did not find any significant improvement with the new proposals and therefore we decided to keep the original set also for the EAF-1 and 2 files.

Table 4. Recommended systematics with their uncertainties.

Reaction	Systematics	Uncertainty[a]
(n,γ)	Kopecky [2]	1.5
(n,p)	Forrest [6]	1.5
(n,h)	Forrest [6]	1.9
(n,α)	Forrest [6]	1.6
(n,n')	Vonach [7]	1.5
(n,2n)	THRES	1.2
(n,3n)	0.8 x THRES	3.0
(n,nα)	0.125 x (n,α)	3.0
(n,d+np)	Forrest [6]	2.0
(n,t+nd)	Forrest [6]	1.6
(n,nt)	-	
(n,nh)	-	
(n,2p)	0.75 x (n,t)	3.0

[a] The uncertainty factors have been derived either from a rigorous error treatment of experimental data and fitted curves [6] or from a simplified graphical treatment (in all remaining cases). The uncertainty (standard deviation) in σ can vary from - σ/f to +fσ .

A remark can be made concerning (n,2n) systematics. By a carefull comparison of all formulae [2,15,16] for new (n,2n) systematics, both against each other and against experimental data, we have realised that the results differ depending on the data set used for fitting (see ref [5]). Thus we have decided at this moment to rely on the original systematics within the THRES code.

4. Renormalizations at 14.5 MeV to experimental data

The main source of 14.5 MeV data in the EAF-1 file has been the extensive compilation of Qaim [23]. In addition some more recent references were used in connection with the special treatment for 102 important reactions [26]. We felt that a large-scale update of the experimental renormalizations is needed. The literature was scanned to find new experimental data at 14 to 15 Mev in the period up to 1990. These data were used to update experimental renormalizations in the EAF-2 file and thus this file reflects the present experimental situation rather well. A listing of all renormalizations is included in the final EAF-2 document [5].
In all new renormalizations, both to systematics and to experimental values, the shape of the excitation curve has been inspected in order to avoid an erroneous application of this procedure for curves with either a steep rise (e.g. (n,3n)) or fall (e.g. (n,2n)) around the 14.5 MeV energy point. The checking procedure was built into our processing code SYMPAL and applied to all renormalizations.

5. Treatment of isomer ratios

Many nuclides have isomer states that are either long lived or which have a different decay mode from the ground state. It is therefore important that in these cases the total reaction cross section for a channel be split by use of a branching ratio so that the cross sections to the ground state and isomer are given separately.
The recommended branching ratios, based on a simplified model calculation with the code CNASH [8] and tabulated in refs. [2,5] have been applied without change for all reactions, this time also including the (n,γ) reaction.
The branching ratio for the capture data was set to a value taken from the systematics for the single-particle emission [8]. In cases where the thermal and resonance regions are included and the thermal experimental isomer ratio exists, this ratio was applied for energies upto E_R.
The branching ratios, predicted from the systematics [8], were recently supported by a theoretical study of Chadwick [24] and the recent, still in progress, irradiation experiment at AEA Harwell on branchings for several long-lived Hf isotopes with high spins of isomeric states [25].

Check and improvement of cross-sections for important reactions

A part of the EAF-1 file was a set of 102 important reactions leading to long-lived products which were evaluated or tested individually [26]. These data are included in the present EAF-2 version, however, no other reactions received special treatment separately in this version. Such action is planned for the future and be based on the results of the sensitivity study (see next paragraph).

Future plans

Further improvements of the EAF-2 file are foreseen. They will be included in the next version, EAF-3, which will be released during the spring of 1992. They can be categorized in five major steps:
1. The issue of completeness needs to be further adressed. The effect of the presence of U and Th impurities in structural materials for fusion reactors has been ignored until now . However, these actinides may be present at level of a few ppm and should be considered [27] in activation and transmutations calculations for low activation materials. To do this the cross section data for 52 actinide targets will be included into the EEF-3 version. The data for these will be generated using THRES, but with (n,γ), (n,f), (n,2n) data taken, wherever available from evaluated files. The remaining (n,γ) reactions will be calculated by the methods used for EAF-2. The missing (n,f) data will either use available data to renormalize data from neighbouring nuclide or will use a simple model calculation.
2. The second step will be the production of the uncertainty file for all cross section data. In the first phase the EAF-3 file will be provided with one-group error file in the data for the (n,x) reactions and with two-group file for the radiative capture data. The latter will cover the thermal and resonance range for capture reactions upto the energy E_R and the remaining part to 20 MeV. To generate the error estimates, both the experimental information and the uncertainties from systematics will be used. Such a data base will enable us to carry out sensitivity studies with the inventory code FISPACT. Also using the dominant nuclides at a

particular time and calculating the sensitivity coefficients of these in conjuction with the uncertainty file, it will be possible to give the uncertainty in the total quantities such as activity.

3. A new code will be selected to replace THRES. This code should be fast and yet include a reliable nuclear model with relatively simple input.

4. An important task will be the improvement of the accuracy of the cross section data base. It may be possible to replace all THRES generated cross sections by a more physically based model, but this activity will be concentrated on the selected amount of important reactions identified in previous studies, such as in ref. [28,29], or from new calculations with EAF-2 data base. The data for these materials will be replaced from the available high-quality libraries as general purpose (EFF/JEF-2, ENDF/B-6 and JENDL-3) files or special files as JENDL-3 activation file or the dosimetry file IRDF-90. For some special cases our own evaluation is not excluded.

5. Finally new reactions, e.g. the sequential reactions discussed by Cierjacks et al. [30], will be included in EAF-3, while gas production cross sections and kerma factors are considered for inclusion.

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