EASY Documentation Series **UKAEA FUS 536**

The European Activation File: EAF-2007 deuteron- and proton-induced cross section libraries

R. A. Forrest

EURATOM/UKAEA Fusion Association, Culham Science Centre,
Abingdon, Oxfordshire, OX14 3DB, UK.

Abstract

The European Activation System (EASY) includes as the source of nuclear data the European Activation File (EAF). A new version of EAF, EAF-2007, has been developed which contains cross section data for deuteron- and proton-induced reactions in addition to the traditional neutron-induced data. This report gives details of the new EAF charged particle libraries. The reason for the addition of these data to EAF is to enable activation calculations to be performed for IFMIF, which is the planned materials test facility.

The EAF-2007 deuteron-induced library contains data for 66,864 reactions, while the proton-induced library contains data for 67,925 reactions.

Contents

Introduction

Neutron-induced reaction cross sections are essential for calculations of the activation of materials that will occur in D-T fusion power plants. ITER is the next-step device that following construction will begin the demonstration that such a power plant is feasible. While ITER will demonstrate the plasma physics and much of the necessary technology, the relatively small neutron fluences mean that the testing of materials to the damage levels expected in a power plant will not be possible. To do this it is proposed that a materials testing facility, IFMIF will be constructed in parallel with ITER. IFMIF will use accelerators to produce intense beams of high energy (40 MeV) deuterons which will strike a flowing lithium target producing an intense neutron field. The neutron spectrum is fusion relevant, but there is a high-energy tail extending up to about 55 MeV, and this fact motivated the extension of the neutron-induced cross sections above 20 MeV that was done for EAF-2005 [1].

The deuterons will themselves cause activation, particularly in the accelerator structure and in the lithium target. The importance of such activation was confirmed using the preliminary deuteron-induced cross section library produced for EAF-2005.1 [2] with calculations of the activation of corrosion elements in the IFMIF lithium loop. Consequently futher work was carried out to improve this library [3] and this is included in EASY-2007 [4]. It is expected that during the initial testing phase on IFMIF deuterons will be replaced by protons or molecular hydrogen ions. This means that to calculate activation a proton-induced reaction library is required. A preliminary library has been produced [5] and this is also included in EAF-2007.

As in the case of the initial deuteron-induced library, the proton-induced library is based purely on model calculations. Extension of SAFEPAQ-II [6] has been necessary to allow proton-induced data to be handled. Experimental data for both deuteron- and proton-induced reactions are available in the EXFOR database and these have been written to CD-ROMs by the NEA Data Bank so that they are accessible to SAFEPAQ-II.

This report details the construction of the deuteron- and proton-induced libraries and gives some examples of the comparion of the data with available experimental data. Unlike the neutron-induced library report [7] a full listing all all the reactions is not given. Since the majority are from TALYS calculations with few modifications the benefit of such a listing is judged to be limited.

Deuteron-induced data

A preliminary deuteron-induced cross section library was produced [3] and used for calculations of the activation of corrosion elements in the IFMIF lithium loop. This library was based on a set of TALYS [8] model calculations. Experimental data for deuteron-induced reactions are available in the EXFOR database and these have been used to determine how well the calculated library fits the measurements. It was realized that some reactions on low-mass targets were not present in the preliminary library, and because other data sources have been generated recently by several groups, it was decided to improve the preliminary library concentrating on the elements that are likely to be found in the accelerator structure.

EAF-2007 d-induced data sets

The TALYS calculations for the preliminary d-induced library released as part of EAF-2005.1 [9] are stored in the TALYS-d data set. The calculations have been repeated by A. Koning (NRG Petten), using improved physics and including additional reactions; these data are stored in the TALYS-6d data source. Another set of calculations made using TALYS but with local parameters rather than the global set used at NRG have been made by M. Avrigeanu (NIPNE) as part of an EFDA Task [10]. These calculations cover only a limited number of targets and are stored in the data set NIPNE-d. Work at ENEA has resulted in a conversion of the Japanese ACSELAM library to a multi-group format that is suitable as input to the ANITA code [11]. This library is also suitable as a data source for the present work and is labeled as ACSELAM-d.

None of these data sets contain data for H or He targets. However, as part of the FENDL/C-2 library [12] reactions relevant to the actual fusion reactions in the plasma have been collected and these contain data for H and He targets, albeit only up to 30 MeV. SAFEPAQ-II [6] has been used to store all these data sources.

EAF-2007 d-induced library

A selection of data source for each reaction was made, based on a comparison of the data sources with experiment. In the majority of cases no data exist and in these cases a judgment based on the quality of the relevant data sources was made. The statistics of the completed library are: 66,864 reactions (compared to 60,688 in EAF-2005.1) of which 66,274 are from TALYS-6d, 219 from NIPNE-d, 346 from TALYS-d, 21 from ACSELAM-d and 4 from FENDL/C-2. A total of 33 renormalizations to EXFOR data have been made as well as many reaction splits to isomeric states. As with EAF-2005.1 there is no uncertainty file.

It is important to stress that in many cases there is a large variation between the various data sources, an example is shown in Figure 1 where there is a factor of four between the data at the maximum. For this reaction the data source chosen for EAF-2007 is NIPNE-d, as this uses a local parameter set which should be the most accurate.

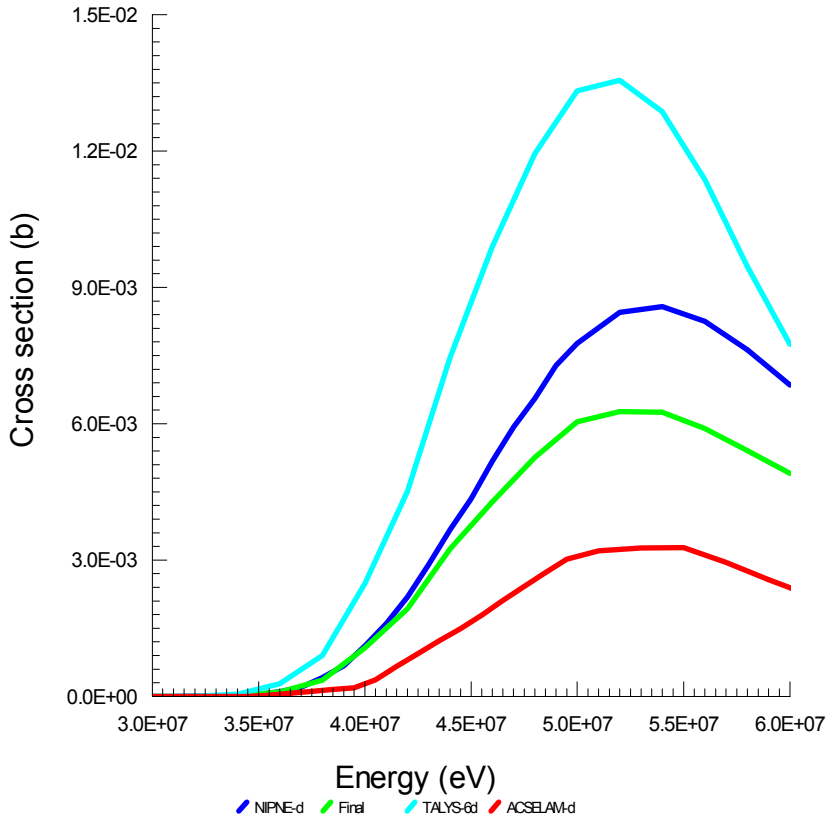

Figure 1. Data for the ^{63}Cu(d,2n2α)^{55}Fe reaction from four sources.

Even when experimental data are available for a reaction the choice of data set can be difficult if the data are discrepant. In such cases usually the most recent data set is assumed correct. An example is shown in Figure 2, where the two experimental data sets are discrepant. TALYS-6d agrees well with the most recent (NRS83) and this source is selected for EAF-2007.

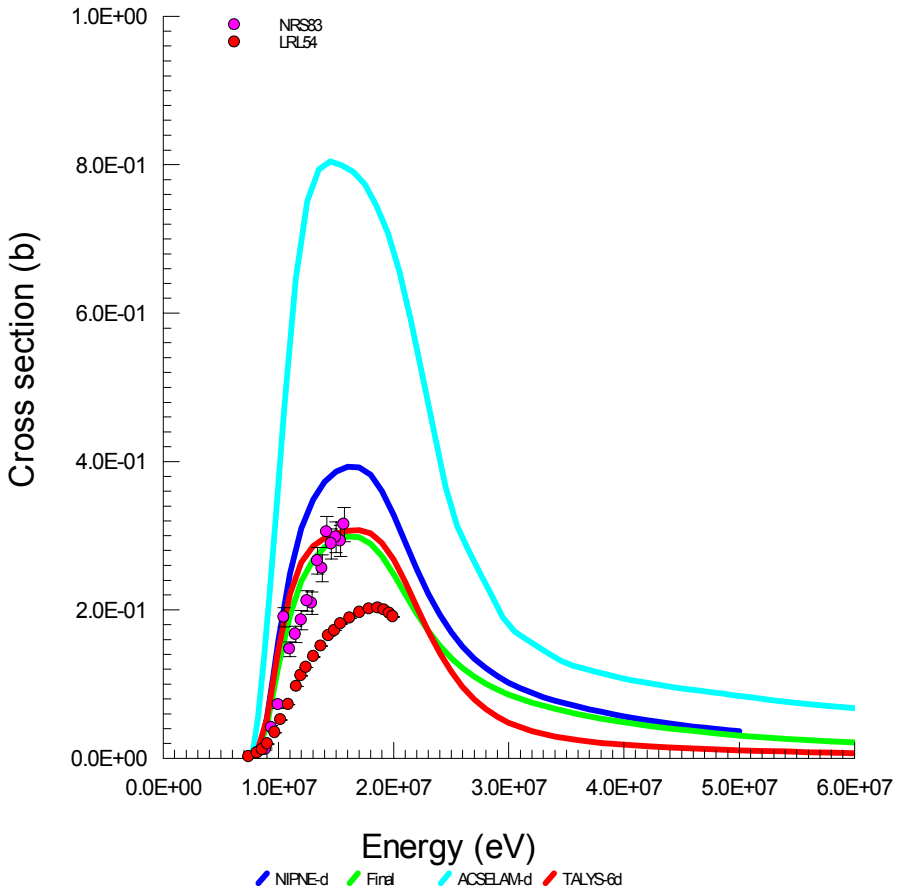

Figure 2. Data for the $^{56}Fe(d,2n)^{56}Co$ reaction from four sources and experimental data from EXFOR.

A further example showing the variation of the data sources and the limited experimental data is shown in Figure 3. It can be seen that the values from ACSELAM-d are very much larger than from the other sources which all agree with the single data point around 20 MeV. Above this energy these three data sources however diverge and the NIPNE-d source is chosen for EAF-2007.

An example of a renormalisation is shown in Figure 4 for the $^{63}Cu(d,3n)^{62}Zn$ reaction. Again the ACSELAM data are much larger than those from the other sources and the measurements. The NIPNE-d data are significantly below the measurements and for EAF-2007 the NIPNE-d data are renormalized to the experimental data at 27.3 MeV.

An example where data from the ACSELAM-d data source are used for EAF-2007 is shown in Figure 5. TALYS is not expected to produce accurate data for low mass targets and as the ACSELEM-d data agree well with the measurements this is chosen as the source for EAF-2007.

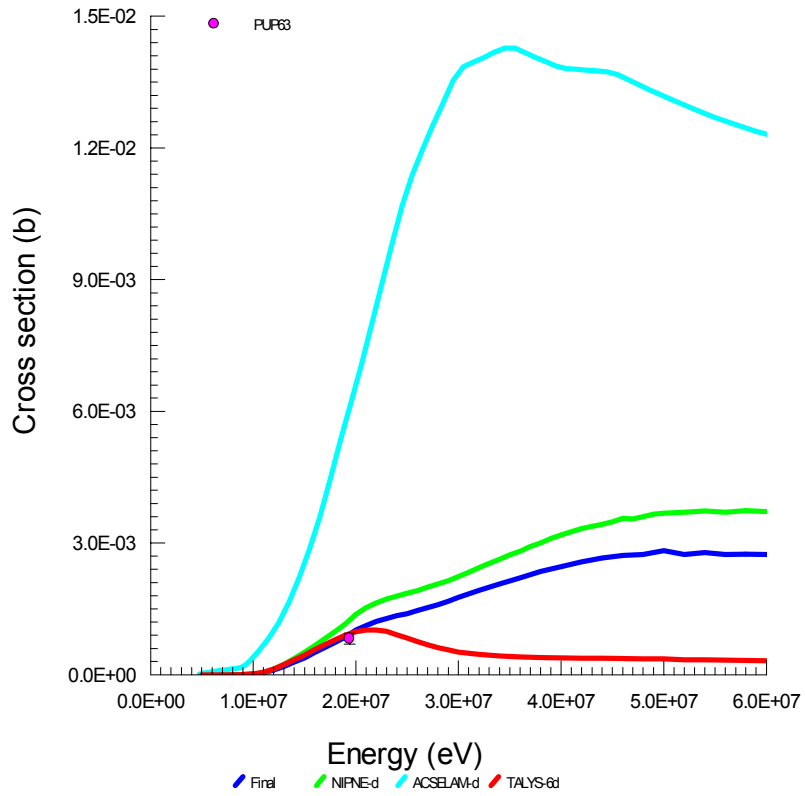

Figure 3. Data for the ^{65}Cu(d,2p)^{65}Ni reaction from four sources and experimental data from EXFOR.

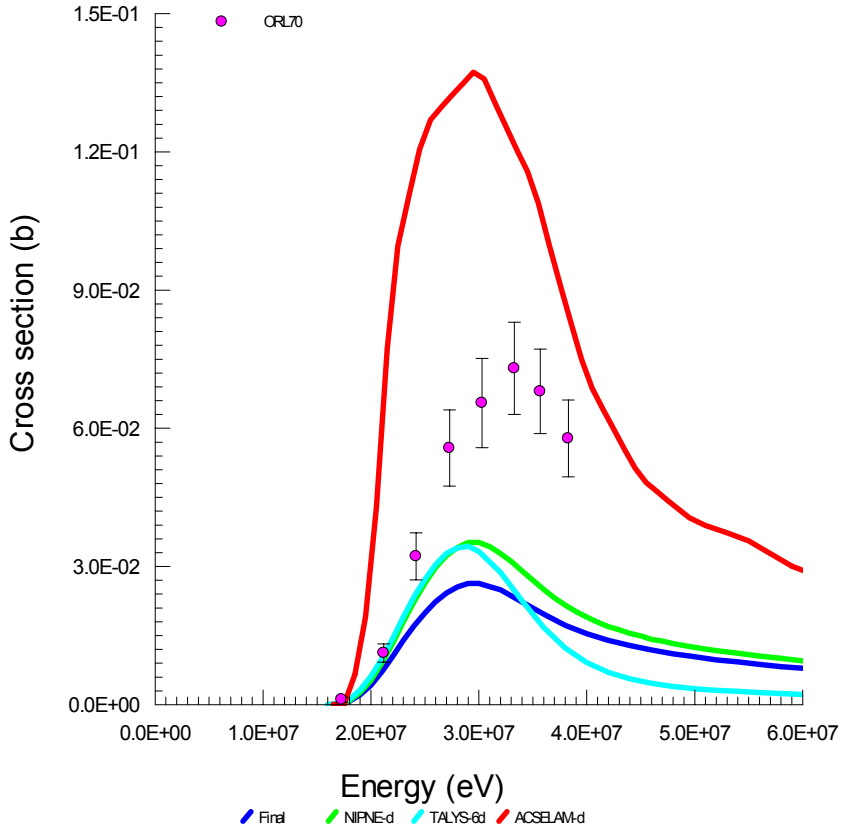

Figure 4. Data for the ^{63}Cu(d,3n)^{62}Zn reaction from four sources and experimental data from EXFOR.

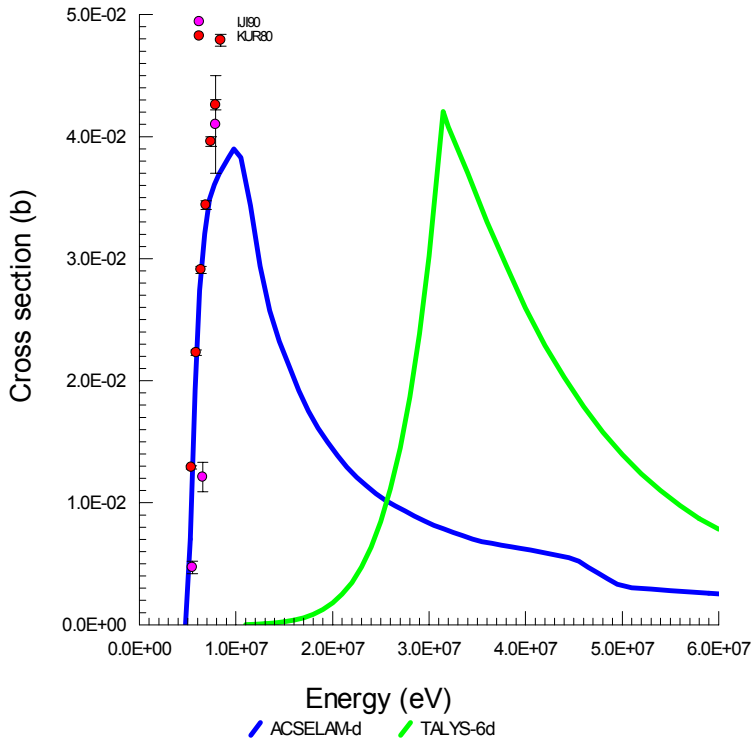

Figure 5. Data for the ^{7}Li(d,2n)^{7}Be reaction from two sources and experimental data from EXFOR.

Two examples of the improvement in the fit to measurements of EAF-2007 over EAF-2005.1 are shown in Figure 6 and Figure 7.

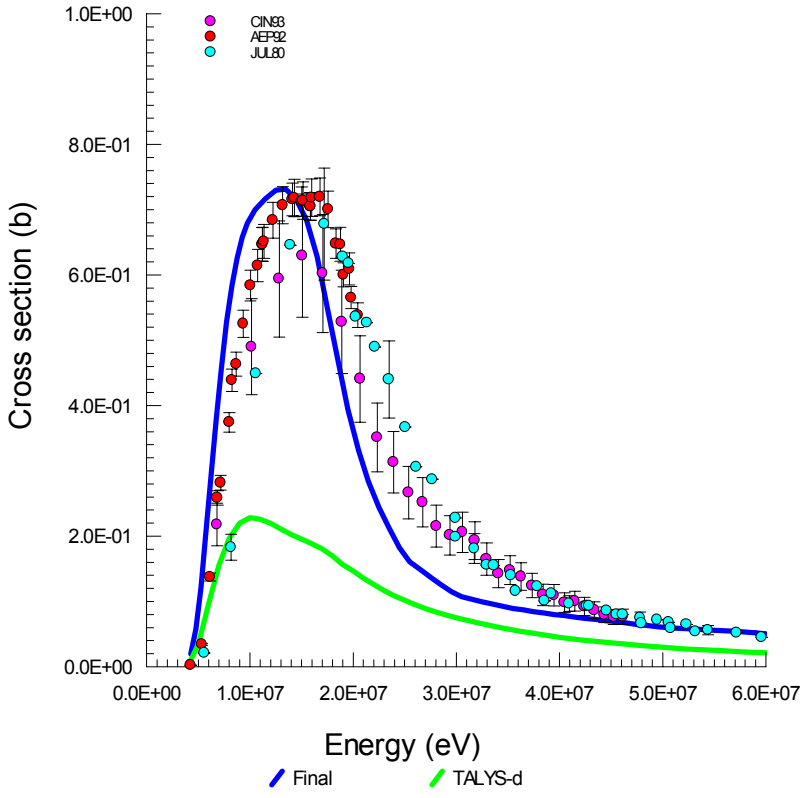

Figure 6. Data for the ^{51}V(d,2n)^{51}Cr reaction from EAF-2007 (Final) and EAF-2005.1 (TALYS-d) with experimental data from EXFOR.

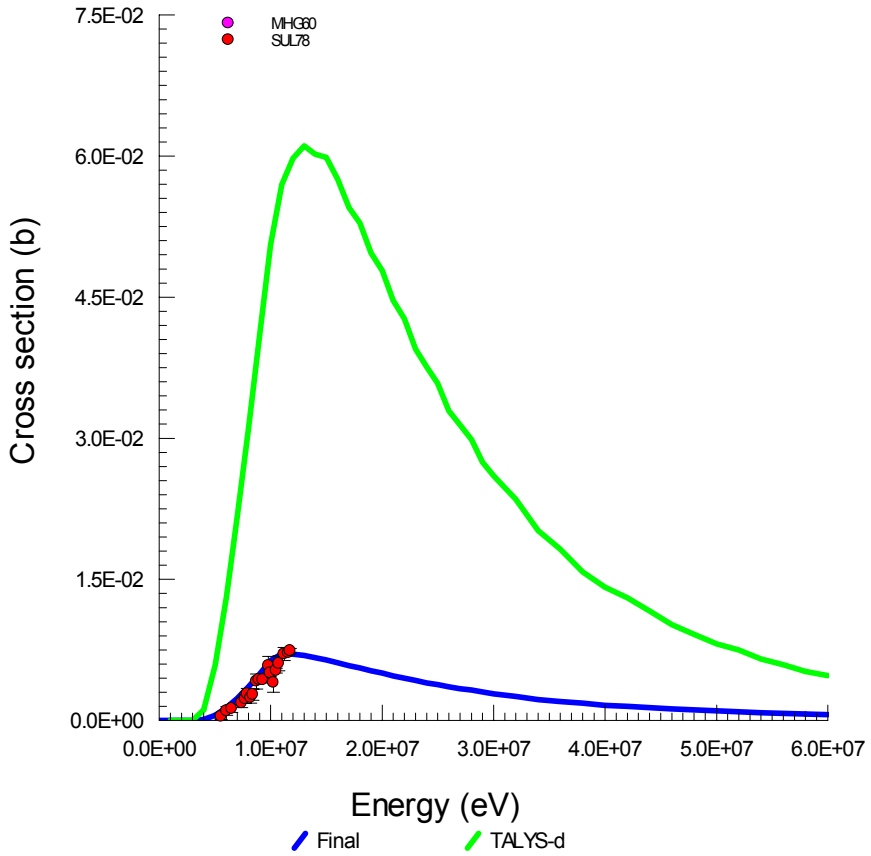

Figure 7. Data for the ^{98}Mo(d,α)^{96}Nb reaction from EAF-2007 (Final) and EAF-2005.1 (TALYS-d) with experimental data from EXFOR.

The 86 reaction types found in the deuteron-induced library are listed in Table 1. Most of reaction data are from the calculations made using the TALYS code, and in addition to the pointwise file, there is a single multi-group library in the VITAMIN-J+ (211-group) flat-weighting format. Details of the multi-group format can be found in the neutron-induced report [6] and the FISPACT user manual [12].

Table 1. Reaction types in EAF-2007 deuteron library

Reaction Type	Number of reactions
d,n	1009
d,d'2n	1069
d,2n	1073
d,3n	1017
d,f	90
d,na	1092
d,n3a	457
d,2na	1095
d,3na	1058
d,np	284
d,n2a	932
d,2n2a	1055
d,d'n	1049

Reaction Type	Number of reactions
d,nt	1074
d,nh	1096
d,d'n2a	460
d,nt2a	408
d,4n	971
d,2np	1049
d,3np	1073
d,n2p	1071
d,npa	1022
d,g	1089
d,p	1049
d,d'	267
d,t	1053
d,h	1074
d,a	1102
d,2a	717
d,3a	264
d,2p	1060
d,pa	813
d,t2a	253
d,d'2a	266
d,d'p	1020
d,pt	719
d,d'a	759
d,5n	863
d,6n	747
d,2nt	1028
d,ta	768
d,4np	1011
d,d'3n	1021
d,d'na	945
d,2npa	1040
d,7n	455
d,8n	169
d,5np	937
d,6np	670
d,7np	233
d,4na	1022
d,5na	900
d,6na	695
d,7na	265
d,d'4n	948
d,d'5n	726
d,d'6n	310
d,3nt	974
d,4nt	853
d,5nt	548
d,6nt	185
d,2nh	1087

Reaction Type	Number of reactions
d,3nh	1076
d,4nh	976
d,3n2p	1066
d,3n2a	1030
d,3npa	1055
d,d't	398
d,d'np	1064
d,npt	968
d,d'nt	813
d,nph	519
d,d'nh	349
d,nth	233
d,nta	990
d,2n2p	1091
d,ph	319
d,d'h	154
d,ha	343
d,4n2p	1027
d,4n2a	946
d,4npa	981
d,3p	292
d,n3p	447
d,3n2pa	560
d,5n2p	758
Total	**66864**

Proton-induced data

EAF-2007 p-induced data set

The only data set for protons considered in the present study is TALYS-6p produced by A. Koning (NRG Petten) using TALYS [8] with global parameters. Consequently the library has no data for H and He targets and there has been no renormalization of data based on experimental measurements.

EAF-2007 p-induced library

The set of reactions in the EAF-2007 proton-induced library was determined by the data available in TALYS-6p. A total of 67,925 reactions are included. As with the deuteron-induced library there is no uncertainty file.

Although there is no direct use of EXFOR data in the construction of the library, comparison of the library data with measurements has been carried out for some reactions to show that the data in the library are suitable for activation calculations. Figure 8 shows data for the reaction ^{55}Mn(p,n)^{55}Fe, and it can be seen that there is reasonable agreement, although the EAF data are larger than the

measurements especially at the higher energies. Figure 9 shows data for the reaction ^{56}Fe(p,n)^{56}Co, and it can be seen that there is reasonable agreement, although the AEP93 data set is very discrepant and should be ignored.

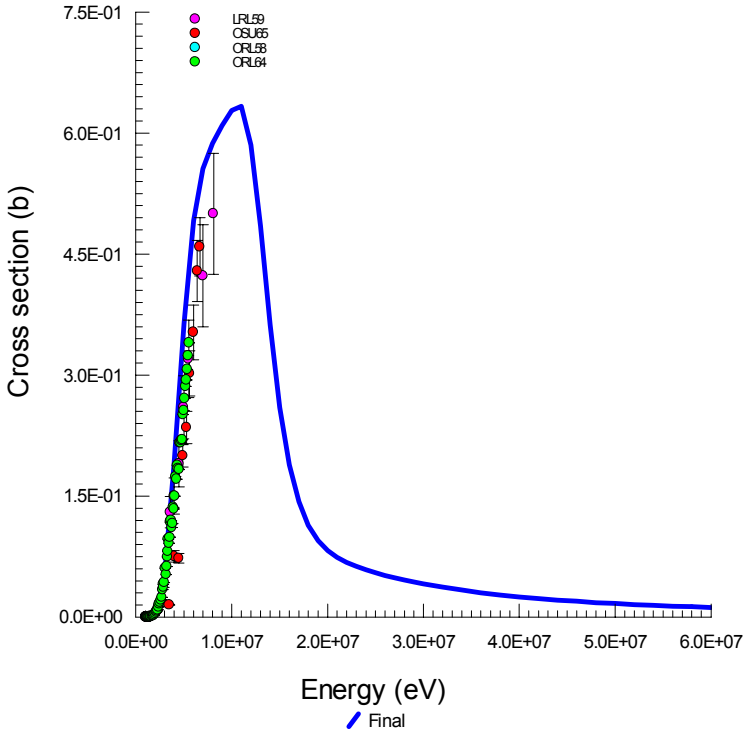

Figure 8. Data for the ^{55}Mn(p,n)^{55}Fe reaction in EAF-2007 with EXFOR data.

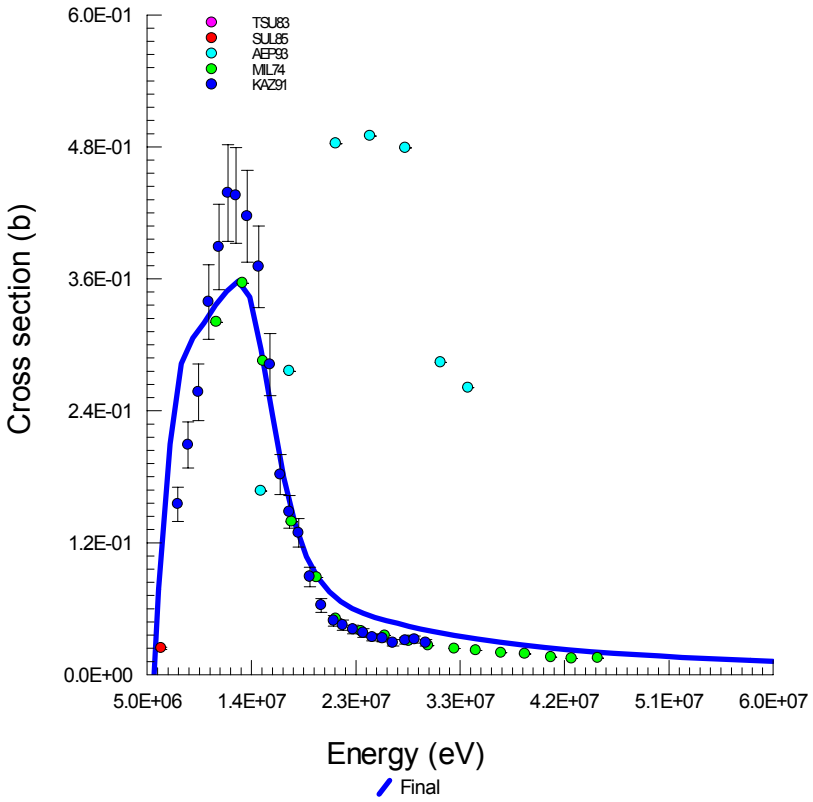

Figure 9. Data for the ^{56}Fe(p,n)^{56}Co reaction in EAF-2007 with EXFOR data.

Figure 10 shows data for the reaction $^{58}Ni(p,\alpha)^{55}Co$, and it can be seen that there is good agreement up to about 30 MeV, the rise in the experimental data above this energy is probably due to the fact that they refer to (p,xα) reactions not just (p,α).

Figure 11 shows data for the $^{56}Fe(p,2n)^{55}Co$ reaction where excellent agreement is seen. A final example is shown in Figure 12, here there is significant disagreement between EAF-2007 and the experimental data, although the main problem seems to be with the experimental data which are discrepant.

The last case emphasises that there are significant improvements that can be made to this preliminary library. Indeed, only a fraction of the available EXFOR data has been studied and it will be necessary to undertake the comparison of EAF-2007 with the experimental data and where necessary add renormalisations in future work.

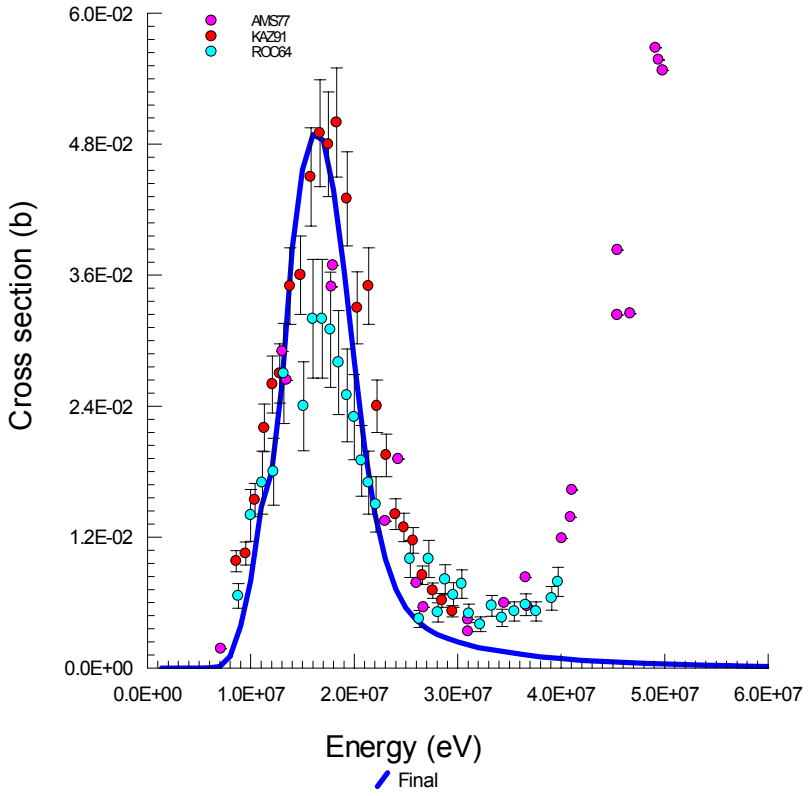

Figure 10. Data for the $^{58}Ni(p,\alpha)^{55}Co$ reaction in EAF-2007 with EXFOR data.

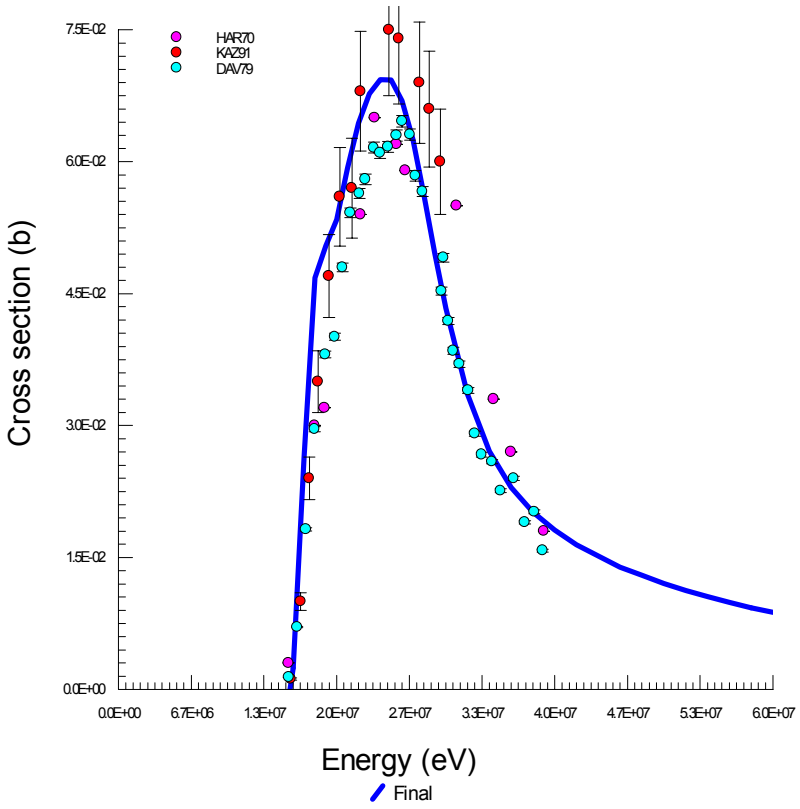

Figure 11. Data for the $^{56}Fe(p,2n)^{55}Co$ reaction in EAF-2007 with EXFOR data.

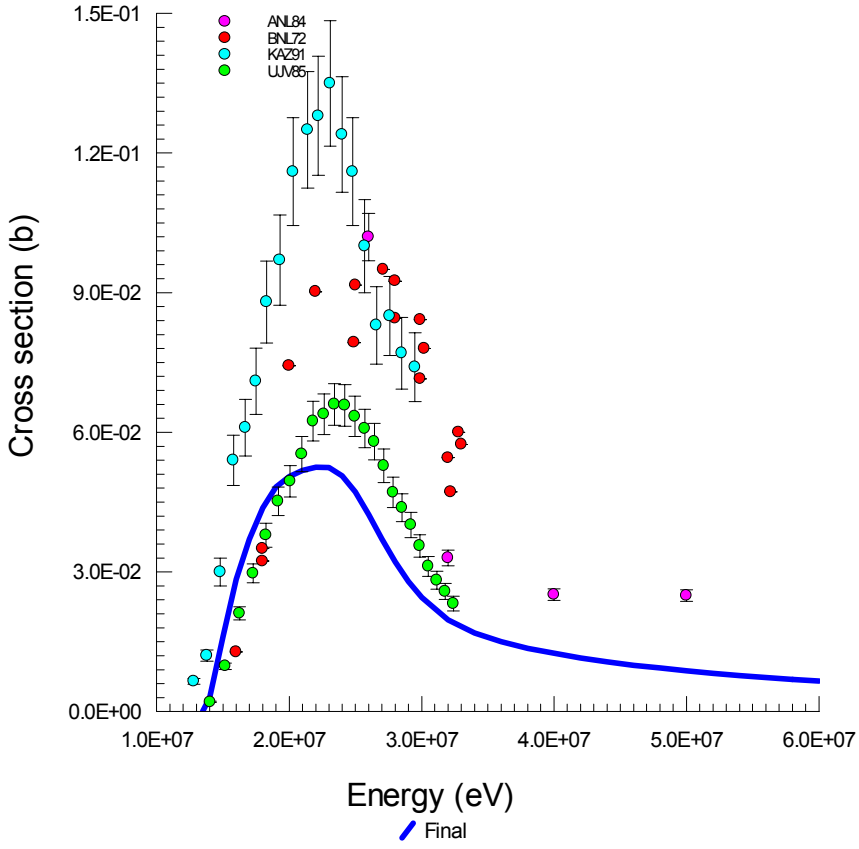

Figure 12. Data for the $^{63}Cu(p,2n)^{62}Zn$ reaction in EAF-2007 with EXFOR data.

The 86 reaction types found in the proton-induced library are listed in Table 2. All reaction data are from the TALYS-6p source, and in addition to the pointwise file, there is a single multi-group library in the VITAMIN-J+ (211-group) flat-weighting format. Details of the multi-group format can be found in the neuton-induced report [6] and the FISPACT user manual [12].

Table 2. Reaction types in EAF-2007 proton library

Reaction Type	Number of reactions
p,n	1028
p,2nd	1033
p,2n	1021
p,3n	982
p,f	90
p,na	1104
p,n3a	491
p,2na	1067
p,3na	1049
p,p'n	836
p,n2a	972
p,2n2a	1029
p,nd	1072
p,nt	1034
p,nh	1093
p,nd2a	468
p,nt2a	412
p,4n	886
p,p'2n	1072
p,p'3n	1034
p,n2p	1103
p,p'na	1044
p,g	1073
p,p'	254
p,d	1050
p,t	1073
p,h	1106
p,a	1099
p,2a	756
p,3a	270
p,2p	1078
p,p'a	926
p,t2a	272
p,d2a	297
p,p'd	1104
p,p't	745
p,da	851
p,5n	810

Reaction Type	Number of reactions
p,6n	654
p,2nt	993
p,ta	804
p,p'4n	991
p,3nd	993
p,nda	1025
p,p'2na	1057
p,7n	401
p,8n	98
p,p'5n	888
p,p'6n	620
p,p'7n	203
p,4na	949
p,5na	871
p,6na	633
p,7na	253
p,4nd	904
p,5nd	668
p,6nd	269
p,3nt	918
p,4nt	790
p,5nt	483
p,6nt	143
p,2nh	1102
p,3nh	1060
p,4nh	985
p,3n2p	1095
p,3n2a	1032
p,p'3na	1028
p,dt	448
p,p'nd	1086
p,p'nt	1044
p,ndt	872
p,p'nh	531
p,ndh	365
p,nth	238
p,nta	984
p,2n2p	1093
p,p'h	354
p,dh	157
p,ha	377
p,4n2p	1013
p,4n2a	913
p,p'4na	966
p,3p	828
p,n3p	745
p,3n2pa	605
p,5n2p	712
Total	**67925**

Conclusions

Cross section data for deuteron- and proton-induced reactions are essential if activation calculations are to be performed for the planned IFMIF device. EASY-2007 contains data for these reactions, although unlike the neutron-induced data almost all of these are from model calculations. In the case of the deuteron-induced library a limited number of reactions have been renormalized to experimental data.

The deuteron-induced library contains data for 66,864 reactions and the proton-induced library contains data for 67,925 reactions. For both libraries the bulk of the data are based on the model code calculations using TALYS with global parameters.

References

[1] RA Forrest, *'The European Activation System: EASY-2005 overview'*, **UKAEA FUS 513**, 2005.

[2] RA Forrest, *'Deuteron-induced activation in the IFMIF lithium loop',* UKAEA report on work performed for EFDA task TW5-TTMI-004, November 2005.

[3] RA Forrest, *'Deuteron-induced cross section library for EAF-2007: Summary',* UKAEA report on work performed for EFDA task TW5-TTMI-004, September 2006.

[4] RA Forrest, *'The European Activation System: EASY-2007 overview'*, **UKAEA FUS 533**, 2007.

[5] RA Forrest, *'Proton-induced cross section library for EAF-2007: Summary',* UKAEA report on work performed for EFDA task TW6-TTMI-004a, September 2006.

[6] RA Forrest, *'SAFEPAQ-II: User manual'*, **UKAEA FUS 454**, Issue 7, 2007.

[7] RA Forrest, J Kopecky and J-Ch Sublet, *'The European Activation File: EAF-2007 neutron-induced cross section library'*, **UKAEA FUS 535**, 2007.

[8] A J Koning, S Hilaire and M C Duijvestijn, *'TALYS: Comprehensive nuclear reaction modeling',* Proceedings of the International Conference on Nuclear Data for Science and Technology – ND2004, Sep. 26 – Oct 1., 2004, Santa Fe, USA, 1154, 2005.

[9] RA Forrest, *'EASY-2005.1: Summary'*, UKAEA report on work performed for EFDA task TW5-TTMN-001, December 2005.

[10] M Avrigeanu, V Avrigeanu, and FL Roman, *'Deuteron-induced activation cross section evaluation for accelerator materials'*, Progress Report to the *EURATOM–MEdC Association* for the time period 2006-01-01 – 2006-06-30.

[11] DG Cepraga, M Frisoni and G Cambi, *'Evaluation of activation inventories and dose rates induced by deuterons*

in the IFMIF accelerator system', EFDA Task No. TW5-TTMI-004, Deliverable 4, Intermediate Report, **FUS-TN-SA-SE-R-146**, July 2006.

[12] AB Pashchenko and H Wienke, *'FENDL/C-2.0: Charged-Particle Reaction Data Library for Fusion Applications Version 1 of March 1997'*, **IAEA-NDS-177**, March 1997.

[13] RA Forrest *'FISPACT-2007: User manual'*, **UKAEA FUS 534**, 2007.

Acknowledgements

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

Disclaimer

Neither the author nor UKAEA accept responsibility for consequences arising from any errors either in the present documentation, or in the EASY-2007 system.

Contact person

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

Dr R A Forrest
EURATOM/UKAEA Fusion Association
D3/1.92 Culham Science Centre
Abingdon
Oxfordshire OX14 3DB
Tel: +44 1235 466586
Fax: +44 1235 466435
e-mail: robin.forrest@ukaea.org.uk
Internet: www.fusion.org.uk/easy2007