Improving activation cross section data with TALYS

Nataliia Dzysiuk[1,a] and Arjan Koning[2]

[1] Nuclear Research and Consultancy Group (NRG), Westerduinweg 3, 1755 LE Petten, The Netherlands
[2] International Atomic Energy Agency, Vienna International Centre, PO Box 100, 1400 Vienna, Austria

Abstract. Needs for accurate (n,x) activation cross sections for fusion technology have been considered with reference to the current status of the TENDL library. The current work is focused on improving activation cross section data for nuclear reactions relevant mainly for fusion and astrophysical needs. The fits have been performed with the TALYS-1.8 code by means of nuclear model parameter variation, mostly for the optical model and level densities, followed by comparison to recent experimental data taken from EXFOR and other evaluated nuclear databases. The updated cross section data are going to be adopted into the new version of TENDL. The improvements have been performed both for differential as well as integral data sets.

1. Introduction

Nuclear data forms the basis of many nuclear technology studies. The area of their applications is expanding and penetrating deeper into various fields of research. One of these is in fusion research where accurate activation cross sections enable efficient development of fusion design concepts. Comprehensive computer modelling of experiments and installations can be achieved using reliable information on cross sections from nuclear data libraries.

The implementation of many research programs requires well-qualified nuclear databases. For instance the Monte Carlo codes must have available a wide range of reliable nuclear reaction cross sections and decay properties for all the materials of interest in the nuclear devices. However despite a large amount of existing nuclear data the problem of inconsistency between various data libraries as well as a lack of those still remains and that requires more efforts and new approaches to solve. Thus the requirements to the quality of those data are quite high. The current work was aimed to verify current requests, following up by improving that set of (n,x) cross sections mainly for the fusion relevant materials [1]. Analysis of available data indicated rather big deviations for more than 100 reaction channels [2] and effort has been applied to perform a better evaluation.

2. TALYS improvements

All calculations of nuclear reaction excitation functions of interest, in the range of (0–30) MeV, have been performed with the TALYS-1.8 code [3]. The fitting procedure of activation cross sections included a variation of the following nuclear model parameters:

- Diffuseness and radius in optical potential
- Model of level densities
- Densities of exciton model constituents
- Pre-equilibrium gamma emission
- Branching ratios
- Probability of α/d/t-particle formation.

Keeping a reasonable balance between competitive channels was the crucial issue. The adjustment was targeted at achieving the best agreement between the latest experimental data, taken from the EXFOR database, and presently calculated TALYS curves. Special attention was paid to fitting the cross sections of isomer production reactions. In this particular case, there was a need to analyze the level structure of the final nucleus thoroughly and to vary the probability of transition between isomer and ground states. Where the information on that transition probability was not given in experimental data tables the values could be estimated. In the fitting procedure it was attempted to fit to the most recent experimental data, to control the shape of excitation curve, and to adjust parameters within acceptable physical limits. In several cases there was a need to study the publications related to measurements in order to understand why some points are outliers when compared general trends. However, in many cases publications did not contain enough details which made process of analysis difficult. One of the most reliable ways of nuclear data validation is a comparison of evaluation to integral data. In the current work, C/E values are used for this purpose, where E – is the real neutron spectrum folded with experimental integral cross section data, C – is the same neutron spectrum folded with the TALYS curve. This ratio can be used as an indicator of the fit quality, and allows for the possibility to analyze each individual channel. In Table 1 there is information on several reactions and C/E values defined using the latest TALYS calculations showing the performed improvements of TENDL-2015. There is a comparison of the latest TALYS fit and data taken from EAF [4] as well as TENDL-2012, 2015 data libraries [5]. In the last column TENDL-2017* is related to a new release of TENDL which is expected at the end of 2017. It is a re-evaluation of TENDL-2015 plus the performed improvements of the cross section fittings. These reactions have been selected

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[a] e-mail: `dzysiuk@nrg.eu`

Table 1. C/E for some reactions.

Reaction	Spectrum	σ(b)	C/E (EAF)	C/E (TENDL 2012)	C/E (TENDL 2015)	C/E (TENDL 2017*)
$^{32}S(n,t)P^{30}$	d-Be	4.13E-03	0.608	0.655	2.770	1.032
$^{34}S(n,p)P^{34}$	fns_5 min	0.0723	0.971	0.996	3.700	1.000
$^{37}Cl(n,\alpha)P^{34}$	fns_5 min	0.0275	0.980	1.305	0.940	1.011
$^{40}Ca(n,t)K^{38}$	d-Be	4.94E-03	0.338	0.571	–	0.996
$^{48}Ca(n,2n)Ca^{47}$	fns_7hours	9.03E-01	0.885	0.885	0.930	1.007
$^{53}Cr(n,p)V^{53}$	sneg_1 cf252_flux_1 rez_DF	5.95E-02 3.06E-04 3.84E-04	0.811 1.880 3.256	0.763 1.699 3.610	0.890 1.610 3.740	0.845 1.792 3.410
$^{61}Ni(n,p)Co^{61}$	fzk_2	1.88E-02	1.722	1.400	1.520	1.002
$^{74}Ge(n,p)Ga^{74}$	fns_5 min	1.32E-03	1.389	1.059	1.110	1.006
$^{82}Se(n,2n)Se^{81}$	fns_5 min	1.00E+00	1.305	1.118	1.180	1.006
$^{144}Sm(n,2n)Sm^{143}$	fns_5 min	1.08E+00	1.165	1.268	1.030	0.980
$^{164}Er(n,2n)Er^{163}$	tud_Er	1.84E+00	0.770	0.828	0.830	0.926
$^{180}Hf(n,p)Lu^{180}$	fns_5 min	1.20E-03	1.961	1.862	0.680	1.091
$^{205}Tl(n,p)Hg^{205}$	fns_5 min	1.93E-03	0.787	0.781	1.430	0.949
$^{206}Pb(n,\alpha)Hg^{203}$	tud_Pb fns_7hours	5.02E-04 1.29E-03	0.761 0.315	0.766 0.317	0.960 0.330	1.018 0.410
$^{51}V(n,\gamma)V^{52}$	sneg_1 cf252_flux_1	1.60E-03 2.80E-03	0.376 0.748	0.505 0.888	– 0.790	1.001 0.962

Energy classification of neutron spectra: fns_5 min, fns_7hours, tud_Pb, fgn_Sn – (3 MeV-14.5 MeV); sneg_1 – (14 MeV – 14.5 MeV); fzk_ss316 – (0.01 MeV – 18 MeV); d-Be – (10 MeV-40 MeV); cf252_flux_1 – (0.2 MeV – 8 MeV). (*) – TENDL-2017 will be released in the end of 2017.

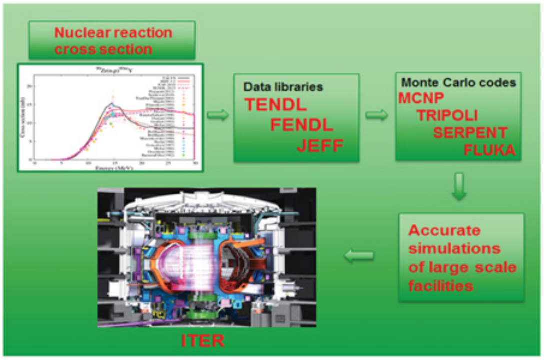

Figure 1. Connections between cross sections and practical applications.

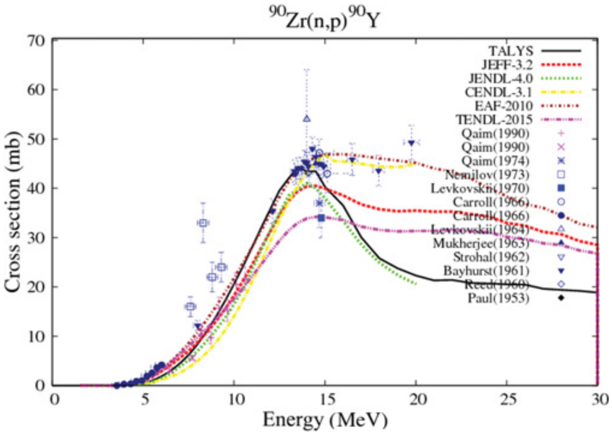

Figure 2. Excitation function for the $^{90}Zr(n,p)Y^{90}$ reaction.

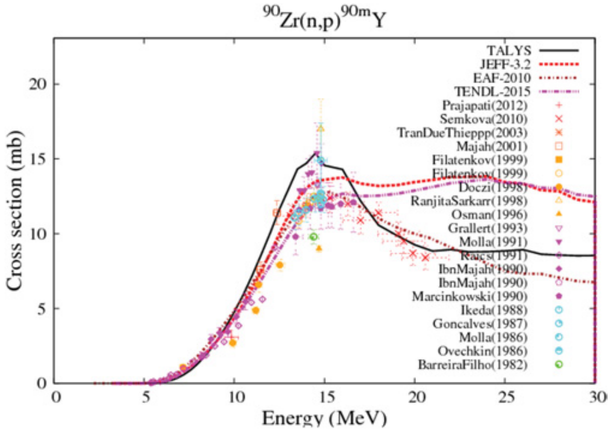

Figure 3. Excitation function for the $^{90}Zr(n,p)Y^{90m}$ reaction.

because for them there are only one or two C/E available in the report of J. Kopecky [6], when there are more values then it is difficult to get an agreement with them all simultaneously and statements about certain improvements are not justified. For example for the $^{51}V(n,\gamma)V^{52}$ reaction it was possible to make validation at two different energy ranges due to availability of corresponding integral experimental data.

Below there is an example of improved fit performed for the $^{90}Zr(n,p)Y^{90}$ and $^{90}Zr(n,p)Y^{90m}$ reactions (Figs. 2, 3). Zirconium is an important construction material therefore such data are of a high priority.

As could be seen in Fig 3, the TALYS curve (black solid line) is in agreement with the latest experimental data taken from EXFOR [7]. On the right side starting from 15 MeV and up TALYS follows the experimental trend and is essentially better than TENDL-2015.

In addition the shape of this excitation function became more physical.

In the case of the capture channel, it was possible to mainly vary the high energy part of the excitation curve. A special attention was paid to the $^{28}Si(n,\gamma)Si^{29}$ reaction since it was mentioned in several literature sources stressing out this certain problem at energies higher than 1 MeV [8]. Now the current evaluation agrees with other evaluated data libraries as well as with the few experimental data at 14 MeV (Fig. 4).

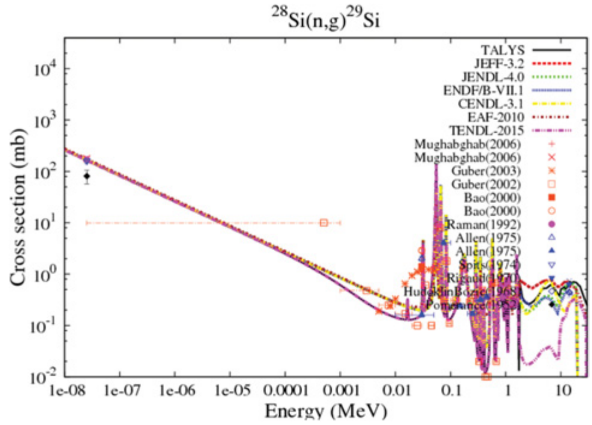

Figure 4. Excitation function for the ^{28}Si(n,γ)Si^{29} reaction.

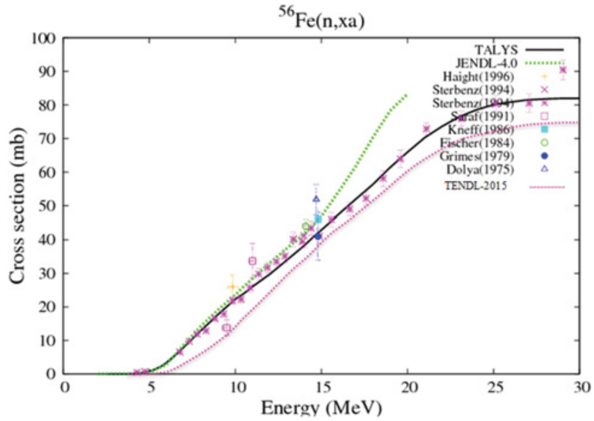

Figure 5. Excitation function for the ^{56}Fe(n,xα) reaction.

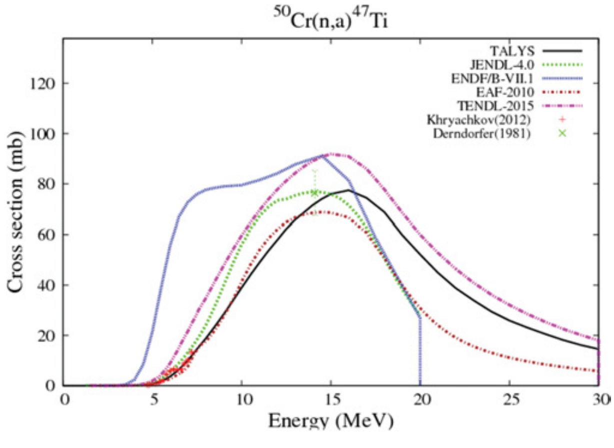

Figure 6. Excitation function for the ^{50}Cr(n,α)Ti^{47} reaction.

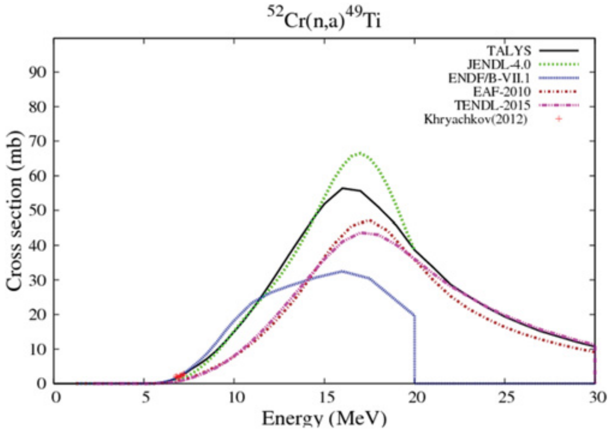

Figure 7. Excitation function for the ^{52}Cr(n,α)Ti^{45} reaction.

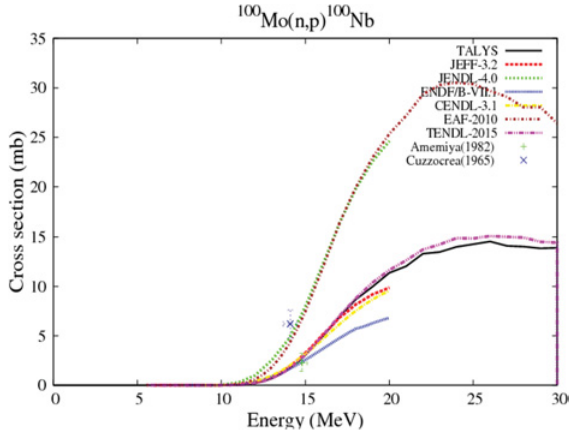

Figure 8. Excitation function for the ^{100}Mo(n,p)Nb^{100} reaction.

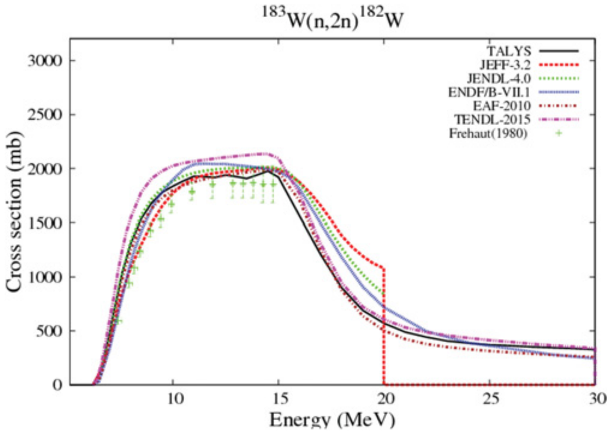

Figure 9. Excitation function for the ^{183}W(n,2n)W^{182} reaction.

Also the problem with iron has been risen in several publications [9]. With respect to those requests in the current study the cross section for the ^{56}Fe(n,xα) reaction was considered and significantly improved (Fig. 5).

It should be emphasized that for (n,α), (n,xα), (n,d), (n,t) reactions it is relevant to take into account the mechanism of formation of particle in output channel. In TALYS this option is implemented by means of a model. Applying the "cstrip" parameter [3] is very efficient to get a better cross section fit for mentioned reactions.

Many new evaluations have been performed for various reactions on chromium isotopes (Figs. 6, 7). Unfortunately the experimental data are very scarce and new measurements are required.

In Fig. 8 there is a fit done for the ^{100}Mo(n,p)Nb^{100} reaction. After studying the papers dealing with those measurements the current evaluation was performed based on the lower experimental point since the other one can be overestimated due to incorrect half-life used for cross section deducing.

In case of the (n,2n) reaction channel it is quite important to choose the level density model. In Fig. 9 there is the evaluation done for the ^{183}W(n,2n)W^{182} reaction. The current fit is in agreement with the only experimental set.

Table 2. MACS.

Reaction	MACS values	
^{32}S(n,γ)S^{33}	EAF-2010 (MACS)	1.224
	TENDL-2015 (MACS)	1.420
	TENDL-2017* (MACS)	1.004
^{44}Ca(n,γ)Ca^{45}	EAF-2010 (MACS)	0.796
	TENDL-2015 (MACS)	0.810
	TENDL-2017* (MACS)	1.075
^{46}Ca(n,γ)Ca^{47}	EAF-2010 (MACS)	1.347
	TENDL-2015 (MACS)	1.160
	TENDL-2017* (MACS)	1.005
^{50}Ti(n,γ)Ti^{51}	EAF-2010 (MACS)	0.769
	TENDL-2015 (MACS)	0.950
	TENDL-2017* (MACS)	1.018
^{54}Fe(n,γ)Fe^{55}	EAF-2010 (MACS)	0.659
	TENDL-2015 (MACS)	0.730
	TENDL-2017* (MACS)	1.040
^{74}Ge(n,γ)Ge^{75}	EAF-2010 (MACS)	0.334
	TENDL-2015 (MACS)	0.960
	TENDL-2017* (MACS)	1.039
^{88}Sr(n,γ)Sr^{89}	EAF-2010 (MACS)	0.918
	TENDL-2015 (MACS)	0.880
	TENDL-2017* (MACS)	1.009
^{92}Mo(n,γ)Mo^{93}	EAF-2010 (MACS)	0.844
	TENDL-2015 (MACS)	0.760
	TENDL-2017* (MACS)	1.002
^{130}Ba(n,γ)Ba^{131}	EAF-2010 (MACS)	0.877
	TENDL-2015 (MACS)	1.090
	TENDL-2017* (MACS)	1.061
^{144}Sm(n,γ)Sm^{145}	EAF-2010 (MACS)	0.951
	TENDL-2015 (MACS)	0.480
	TENDL-2017* (MACS)	1.006
^{186}W(n,γ)W^{187}	EAF-2010 (MACS)	0.842
	TENDL-2015 (MACS)	0.850
	TENDL-2017* (MACS)	1.007
^{207}Pb(n,γ)Pb^{208}	EAF-2010 (MACS)	0.740
	TENDL-2015 (MACS)	1.190
	TENDL-2017* (MACS)	1.001

In addition to a qualitative fit of the (n,γ) reaction channel which is relevant for fusion, the values of Maxwellian Average Cross Section (MACS) at $kT = 30$ keV were calculated with TALYS as well. Such analysis was done based also on information obtained from the report [10]. Afterwards the ratio between the experimental MACS value taken from the KADoNiS data library [11] and value calculated with TALYS, what refers to TENDL-2015 plus improvements, is given in Table 2. For light nuclei it is difficult to get a trustworthy and exact value because 30 keV is in the resonance range, while for heavier nuclei the value could be obtained with increased accuracy. It can be seen that for many reactions the ratio is very close to 1.00, which quantitatively proves the TALYS features. This kind of data is highly important for nuclear astrophysics.

3. Conclusion

A set of activation cross sections have been improved using the TALYS-1.8 code. These data will serve as input file for generation a new release of TENDL data library (TENDL-2017). In total more than 100 reactions of different types have been under consideration. Mainly it concerned fusion relevant materials such as Fe, Cu, Mo, Mn, Cr, Si, Ti, W, Zr, Pb, Na and others which can be considered as impurities. In the most important cases, good agreement between current TALYS predictions and experimental data, taken from a wide range of measurement techniques, was achieved. Data validation was done by means of comparing to integral measurements, and C/E values of approximately 1.00 was calculated for 40 reactions.

Below there is a shortened list of considered reactions in this current work: ^{23}Na(n,γ)Na^{24}, ^{24}Mg(n,γ)Mg^{25}, ^{50}Ti(n,γ)Ti^{51}, ^{51}V(n,γ)V^{52}, ^{54}Fe(n,γ)Fe^{55}, ^{58}Fe(n,γ)Fe^{59}, ^{54}Mn(n,γ)Mn^{55}, ^{55}Mn(n,γ)Mn^{56}, ^{58m}Co(n,γ)Co^{59}, ^{59}Co(n,γ)Co^{60}, ^{63}Cu(n,γ)Cu^{64}, ^{65}Cu(n,γ)Cu^{66}, ^{74}Ge(n,γ)Ge^{75}, ^{27}Al(n,2n)Al^{26m}, ^{36}S(n,2n)S^{35}, ^{46}Ti(n,2n)Ti^{45}, ^{48}Ca(n,2n)Ca^{47}, ^{50}Cr(n,2n)Cr^{49}, ^{52}Cr(n,2n)Cr^{51}, ^{56}Fe(n,2n)Fe^{55}, ^{60}Ni(n,2n)Ni^{59}, ^{72}Ge(n,2n)Ge^{71}, ^{114}Sn(n,2n)Sn^{113}, ^{120}Sn(n,2n)Sn^{119}, ^{140}Ce(n,2n)Ce^{139}, ^{34}S(n,α)Si^{31}, ^{40}Ca(n,α)Ar^{37}, ^{48}Ca(n,α)Ar^{45}, ^{46}Ti(n,α)Ca^{43}, ^{50}Cr(n,α)Ti^{47}, ^{52}Cr(n,α)Ti^{49}, ^{56}Fe(n,p)Mn^{56}, ^{67}Zn(n,p)Cu^{67}, ^{90}Zr(n,p)Y^{90g}, ^{94}Mo(n,p)Nb^{94}, ^{95}Mo(n,p)Nb^{95}, ^{116}Sn(n,p)In^{116}, ^{117}Sn(n,p)In^{117}, ^{183}W(n,2n)W^{182}, ^{187}Re(n,2n)Re^{186g}, ^{49}Ti(n,np)Sc^{48}, ^{28}Si(n,p)Al^{28}, ^{55}Mn(n,α)V^{52}, ^{60}Ni(n,p)Co^{60m}. In order to increase the reliability of the evaluation procedure, more accurate experimental data is required.

References

[1] R.A. Forrest, "Nuclear Science and Data Needs for Advanced Nuclear Systems",*(Energy Procedia), Asian Nuclear Prospects* (2010)

[2] N. Dzysiuk, A. Koning, JEFF-presentation, EFFDOC-1288 (2016)

[3] A.J. Koning and D. Rochman, "Modern nuclear data evaluation with the TALYS code system", Nuclear Data Sheets **113**, 2841 (2012)

[4] J.-Ch.Sublet, L.W.Parker, J.Kopecky, EASY Documentation Series, CCFE-R(10)05 (2010)

[5] `https://tendl.web.psi.ch/tendl_2015/tendl2015.html`

[6] J. Kopecky, "JRR report-X" (November 2015)

[7] `https://www-nds.iaea.org/exfor/exfor.htm`

[8] P. Sauvan, M. Garcia, J. Sanz, F. Ogando, Presentation JEFF meeting, EFFDOC-1277 (Dec. 2015)

[9] S.P. Simakov, A. Koning, A.Yu. Konobeev, TM "Nuclear Reaction Data and Uncertainties for Radiation Damage", IAEA13-17 June (2016)

[10] J.Ch. Sublet, M. Fleming, J. Kopecky, M. Gilbert, D. Rochman, A. Koning, UKAEA-R(15) 35, November 2015

[11] `http://www.kadonis.org/`

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