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ABSTRACT

This report presents the use of the kT = 30 keV Maxwellian averaged cross sections (MACS) to test and validate the capture cross section curve. The performance of FENDL-3/A library has been tested and compared with recommended MACS data from the KADoNiS compilation and with data from ENDF/B-VII.1 and TENDL-2012 libraries.

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Contents

1. Introduction

The validation of capture cross sections has been recently extended by integral measurements such as resonance integrals, the Maxwellian spectrum at 30 keV and the fission spectrum from ^{252}Cf source. These data have been applied for validation of activation library EAF-2010 [1] adopted for FENDL-3/A [2] and published in Refs. [3,4].

In this report the performance of the *Maxwellian averaged cross section (MACS)* used in these validation procedures is described. The 30 keV cross sections have been extensively studied within the astrophysics community, in particular by the Karlsruhe group, resulting in two compilations, published in 1987 [5] and 2000 [6]. In both compilations the experimental results for stable targets between H and Bi have been surveyed, renormalized to a cross section standard (^{197}Au) and stored as a set of recommended Maxwellian averaged cross sections (MACS) at kT = 30 keV. These averaged cross sections are derived from either activation experiments in which the neutron spectrum has a shape close to the Maxwell-Boltzmann spectrum (usually from the ^{6}Li (p,n) reaction) or from TOF experiments. Details of these measurements, applied corrections and normalizations as well as the calculations are described in Refs. [7,8]. In cases where no experimental information was available the statistical model calculations with the NON-SMOKER code [9] were used and also included as the recommended cross sections. This data base is regularly updated with new measurements.

The latest release of this compilation in electronic format is from 2009 and can be found on the KADoNiSv0.3 website [10]. It includes the most recent recommended MACS cross sections for kT = 30 keV, calculated with Eq. (1) using the analytical form of the Maxwell-Boltzmann neutron spectrum:

$$\langle\sigma v\rangle/v_T = \frac{2}{\sqrt{\pi}}\frac{\int \sigma(E_n)E_n\exp(-E_n/kT)dE_n}{\int E_n\exp(-E_n/kT)dE_n} \quad (1)$$

Reference [8] defines the experimental cross section used in this calculation by Eq. (2).

$$\frac{\langle\sigma v\rangle}{v_T} = \frac{2}{\sqrt{\pi}}\sigma_{exp}\,(E_n) \quad (2)$$

The factor $(2/\sqrt{\pi}) = 1.128$ comes from the normalization of the Maxwell-Boltzmann equation using the mean thermal velocity and $\sigma_{exp}(E_n)$ is the average integral Maxwell-Boltzmann cross section deduced from the experiment.

In EAF integral validation (see e.g. Ref. [11]) the neutron source averaged cross section $<\sigma>$ is the effective value of the reaction cross section for a given neutron spectrum, with E_1 and

E_2 as the energy limits, $\sigma(E)$ an energy dependent reaction cross section in a group structure (usually Vitamin-J 175 groups) and $\varphi(E)$ the neutron spectrum in the same group structure, usually determined experimentally. The formula has a form of

$$< \sigma > = \frac{\int_{E1}^{E2} \sigma(E)\varphi(E)dE}{\int_{E1}^{E2} \varphi(E)dE} \quad \text{or} \quad < \sigma > = \sum_1^n \sigma_i \, \varphi_i / \sum_1^n \varphi_i \tag{3}$$

This equation is used in the processing code SAFEPAQ-II [12], which calculates $<\sigma>$ with $\sigma(E)$ taken from the studied library, while for MACS the spectrum $\phi(E)$ has the analytical form of a Maxwell-Boltzmann (MB) spectrum for E_n = 30 keV. This cross section is further denoted as $<\sigma_{30keV}>$ and defined as

$$< \sigma_{30keV} > = \frac{2}{\sqrt{\pi}} < \sigma > \tag{4}$$

The definition of $\sigma_{exp}(E_n)$ in Eq. (2) and $<\sigma>$ from Eq. (3) are the same with one difference, namely that $<\sigma>$ is a quantity based on the evaluated $\sigma(E)$ from the studied library without any additional normalization, while in $\sigma_{exp}(E_n)$ the cross section $\sigma(E_n)$ is based on an evaluation normalized to the 30 keV integral experiment. In both cases the cross section is folded with an analytically calculated MB neutron spectrum.

2. Data analysis

The global performance of MACS has not yet been tested with recent libraries. Three libraries, the activation library FENDL-3/A, the general purpose library ENDF/B-VII.1 [13,14] and the recent TENDL-2012 [15,16] have therefore been used to test the global performance of C/E values. For the FENDL-3/A library the cross section $<\sigma>$ and $<\sigma_{30keV}>$ values have been calculated with the processing code SAFEPAQ-II, while MACS values for ENDF/B-VII.1 and TENDL-2012 were taken from Refs. [13,15]. The resulting C/E distributions as a function of the mass A are shown in Figs. 1-3 with their average mean values. The adopted average cross sections were calculated with Eqs. (1) and (4) and for recommended MACS data the KADoNiS compilation [10] has been used. For this comparison only measured total cross sections (not calculated) MACS data from Ref. [10] have been used. The number of 248 targets was chosen, based on the content of ENDF/B-VII.1. This enables a direct comparison of the same group of data among the studied libraries.

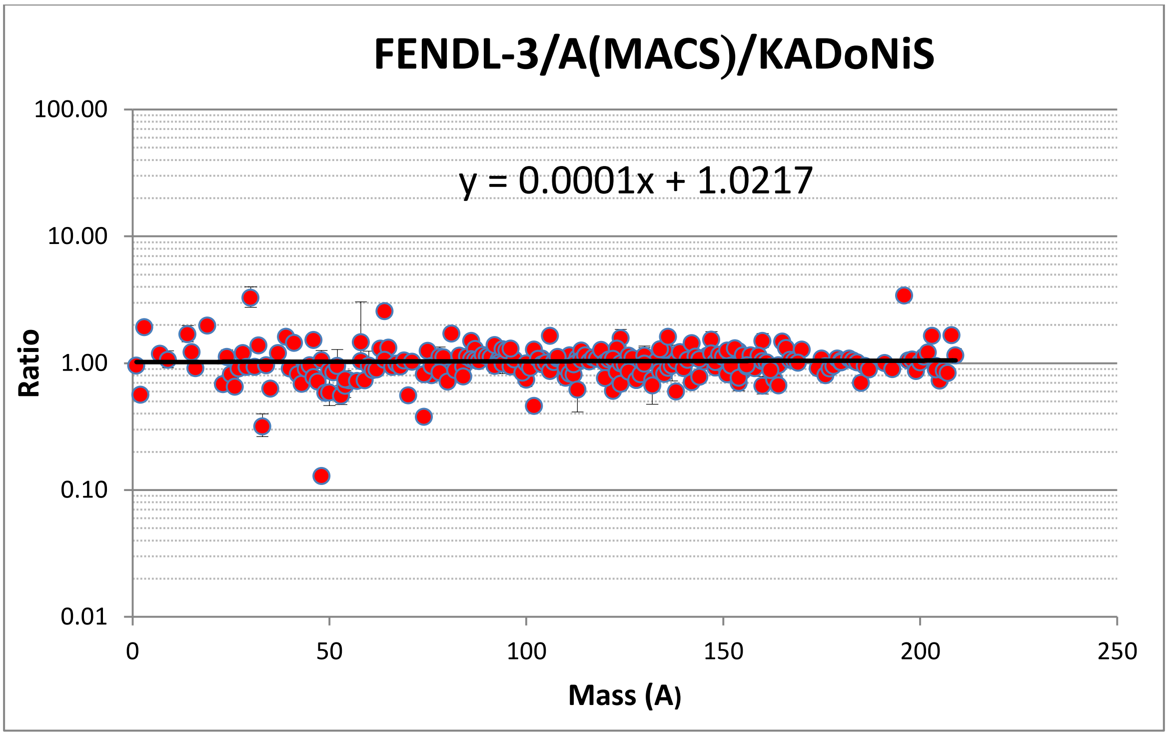

Fig.1: *C/E (MACS) ratio derived from FENDL-3/A data using Eq. (4).*

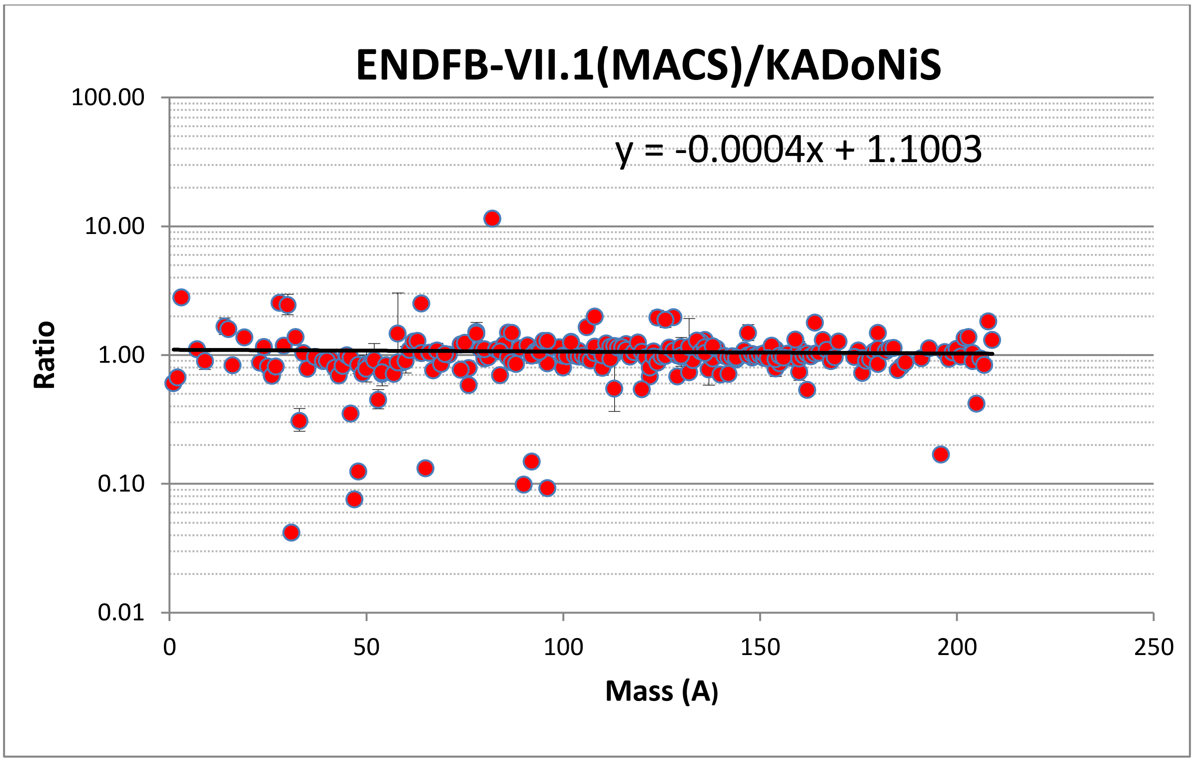

Fig.2: *C/E (MACS) ratio of ENDF/B-VII.1 data taken from [12,13] using Eq. (1).*

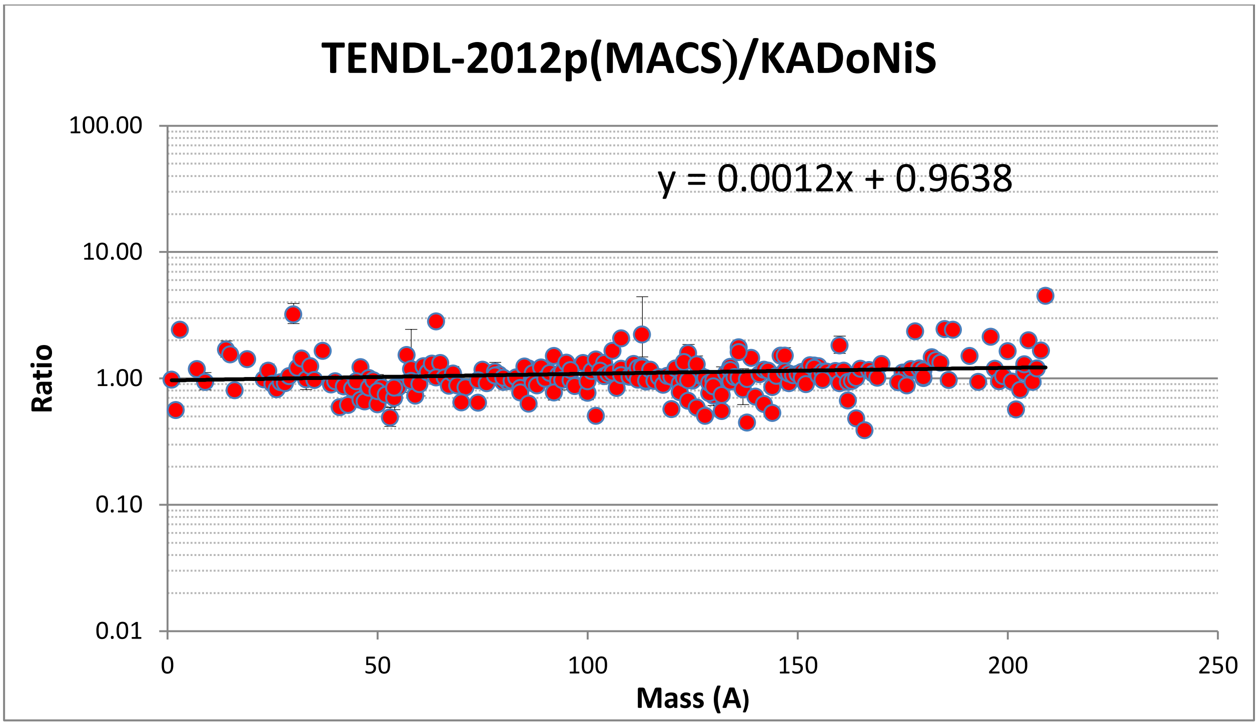

Fig.3: *C/E (MACS) ratio of TENDL-2012 using Eq. (4).*

In order to check the integration methods in preprocessing codes applied to ENDF/B-VII.1(LINEAR) and/or TENDL-2012 and FENDL-3/A libraries (SAFEPAQ-II using group structure data) with Eq. (3) and (4), the MACS values have been recalculated for ENDF/VII.1 with SAFEPAQ-II. The results were almost identical and remained within 0.5% scatter. The resulting averaged linear trend lines of C/E ratios are shown in Table 1.

Table 1. C/E trend lines calculated for 248 cross section entries of ENDF/B-VII.1 and for entries with 0.5 > |C/E| > 2 outliers removed (see Table 2).

Data source	C/E Trend line 248 targets	C/E Trend line 0.5 ≤|C/E| ≤ 2 data only
FENDL-3/A	(0.0001A + 1.0217) ± 0.05	(-6.00E-7A + 1.0175) ± 0.05
ENDF/B-VII.1	(-0.0006A + 1.1003) ± 0.05	(0.0003A + 1.0029) ± 0.05
TENDL-2012	(0.0012A + 0.9638) ± 0.05	(0.0011A + 0.9383) ± 0.05

The studied libraries are rather consistent in their response to the MACS data, which is demonstrated in a similar behaviour of the C/E ratio as a linear function independent of *A* for FENDL-3/A and ENDF/B-VII.1, while a slightly increasing trend with *A* has been detected for TENDL-2012. The C/E values for TENDL-2012 increase from 0.97 to 1.20, for *A* = 10 and 200, respectively. Mean trend values of C/E for MACS/KADoNiS cross sections are expected to be around unity, which is true for FENDL-3/A and TENDL-2012, considering the uncertainty of about 5% of the derived trend lines, while the result for ENDF/B-VII.1 is about 10% larger. In order to test whether the trend values are influenced by large data outliers, the analysis was repeated with the exclusion of values larger than an arbitrarily chosen limit of 0.5 > |C/E| > 2. The list of these deleted values is shown in Table 2.

Table 2. List of targets with 0.5 > |C/E| > 2 values removed from the analysis. 0.1 > |C/E| > 10 in bold italics

Target	C/E FENDL-3/A	C/E ENDF/B-II.1	C/E TENDL-2012
He-3		***0.003***	2.42
Si-30	3.07	2.44	3.20
P-31		0.42	
S-33	3.17	0.31	
Ca-45		0.35	
Ca-48	0.13	0.12	
Ti-47		***0.08***	
Ni-64	2.57	2.51	2.34
Cu-65		0.13	
Ge-74	0.38		
Kr-82		***11.40***	
Zr-90		0.10	
Zr-92		0.15	
Mo-96		***0.09***	
Cd-108			2.07
Cd-13m			2.22
Ba-148			0.45

Target	C/E FENDL-3/A	C/E ENDF/B-II.1	C/E TENDL-2012
Nd-147			2.34
Er-164			0.48
Er-166			0.38
Re-185			2.46
Re-187			2.42
Hg-196	3.41	***0.17***	2.12
Tl-205		0.42	
Bi-209			4.50
Total #	**6**	**15**	**13**

The result of the trend analysis with the reduced number of targets is shown in the third column of Table 1. The global agreement with KADoNiS data very is satisfactory for FENDL-3.2/A and ENDF/B-VII.1, while TENDL-2012 shows a small global underestimation. The new value for ENDF/B-VII.1 shows the influence of extreme outliers on the trend analysis. The largest number of outliers is in ENDF/B-VII, which may explain the 10% deviation of the trend line value, influenced mainly by the large C/E of ^{82}Kr. The reason for that is shown in Fig.4, where it can be seen that the resonance region in ENDF/B-VII.1 is obviously wrong.

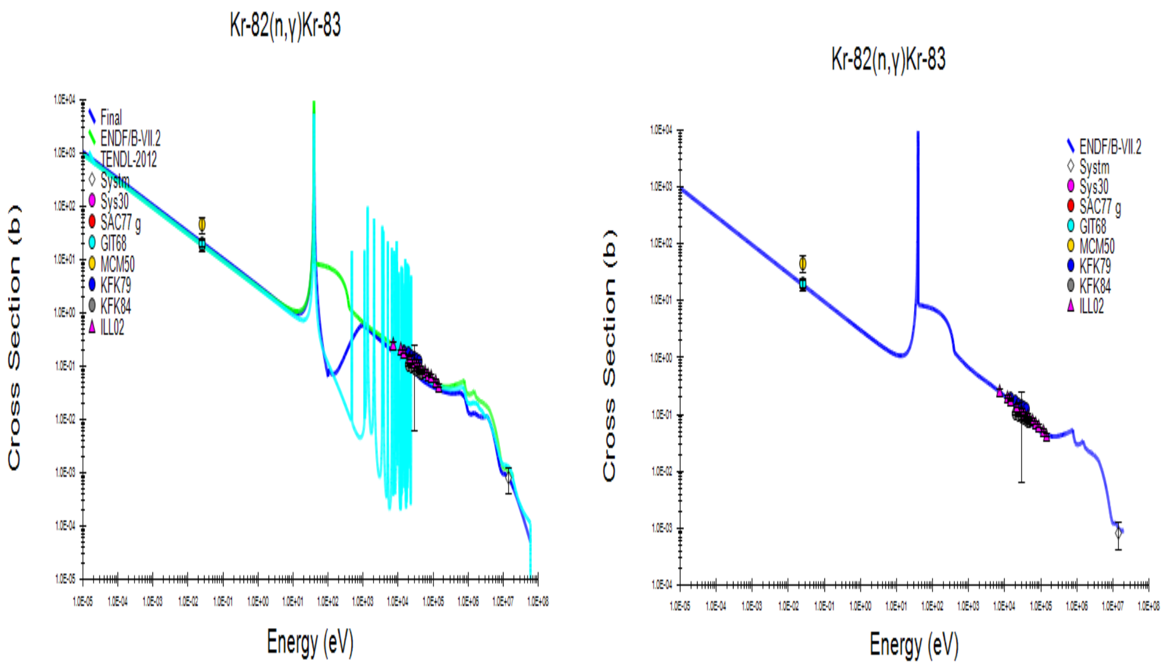

Fig.4: *^{82}Kr(n,γ) reaction with a wrong resolved resonance region in ENDF/B-VII.1 (see the right plot). 'Final' stands for FENDL-3/A data.*

For three targets (^{30}Si, ^{64}Ni and ^{196}Hg) all three libraries have discrepant C/E values and this may suggest some common problem in evaluations. As an example we discuss the ^{196}Hg target (see Fig. 5). The ENDF/B-VII.1 excitation curve is obviously too low, the other two evaluations show a small overestimation in the smooth unresolved resonance region which needs to be corrected. This example demonstrates the sensitivity of such analysis to detect deviations.

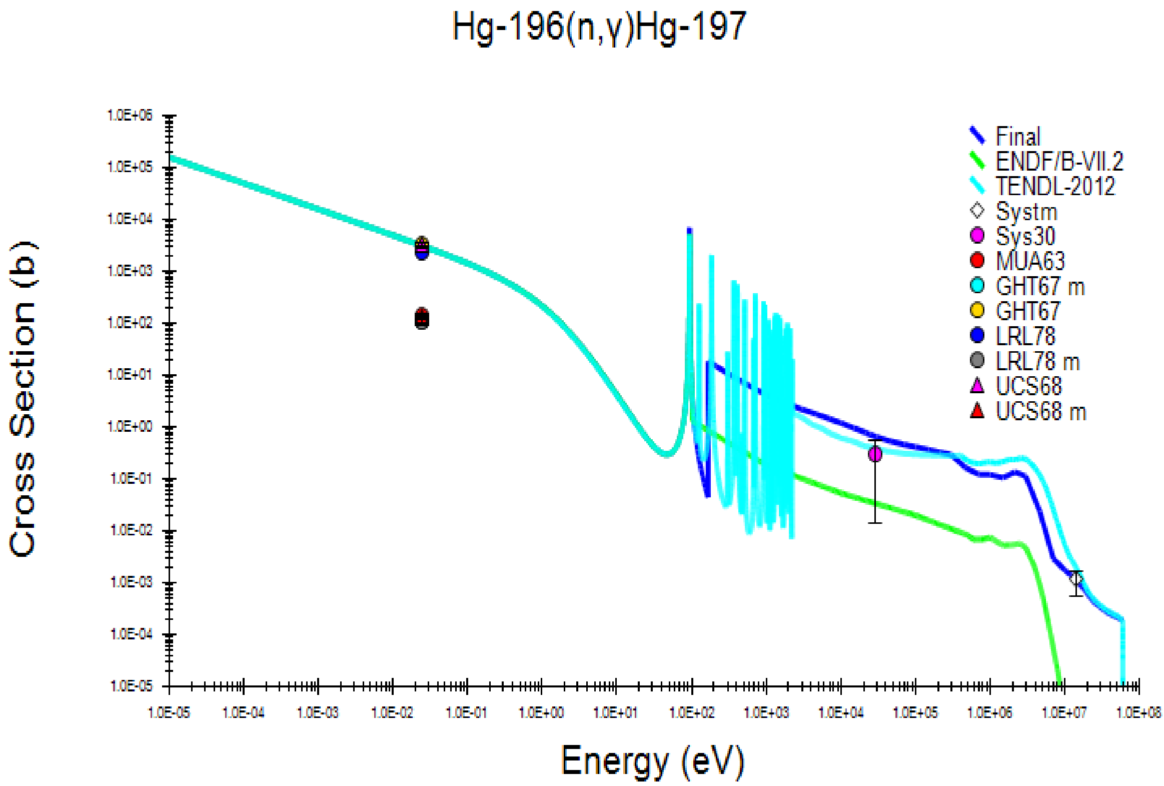

Fig. 5: *The ^{196}Hg(n,γ) reaction, note the strong underestimation of ENDF/B-VII.1 data.*

3. Conclusions

1. The KADoNiS data base is important information for capture cross section validation in the whole mass range. While for lower masses (A < 100) the C/E value is primarily influenced by the resolved resonance region, while the smooth unresolved region of the cross section is relevant for heavier targets.

2. The capture cross section data in the energy region of a 30 keV Maxwellian spectrum are in agreement within 10% with the recommended KADoNiS values for all three studied libraries. The performance in terms of C/E trend can be seen from the following table:

Library	**C/E (248 targets)**	**Outliers removed**
FENDL-3/A	1.0217 ± 0.05	1.0175 ± 0.05
ENDF/B-VII.1	1.1003 ± 0.05	1.0092 ± 0.05
TENDL-2012	0.9638 ± 0.05	0.9383 ± 0.05

   The removal of obvious outliers (with 0.5 > |C/E| > 2) has the largest influence for the ENDF/B-VII.1 library, while the smallest number of outliers (5 against 13 and 15, respectively) and therefore their influence on the C/E trend was found for FENDL-3.2/A. The performance of FENDL-3/A seems to be the best.

3. The good performance of FENDL-3.2/A data in the MACS validation test supported the application of these data for validation for all targets. We used two comparisons, for targets provided with KADoNiS data (both measured and calculated) the C/E comparison of MACS cross sections was interpreted as quasi-monoenergetic data σ(30 keV) (for details see Ref. [4]) and for all targets the C/S comparison of σ(30 keV) was derived from the cross section systematic [18]. The results are shown in Fig. 6. In the left hand part of this figure, the C/E histogram for 328 reactions shows excellent agreement with MACS data, these reactions are usually also provided with other differential data and can be considered as validated. The tail of data points with C/E < 0.5 are for reactions with the 30 keV energy point in the middle of the resolved resonance region and in such cases the 30 keV cross section cannot be compared with average MACS data.

   More interesting is the second plot, in the right hand part of the figure. It addresses all targets which for the majority are without any experimental information. It shows that despite the simplification applied in the derivation of the systematic and in the evaluation of the excitation curve, based only on phenomenological information, the agreement is rather satisfactory. The major trend of 770 reactions is again well centered at unity and the tail for small C/E values arises for the same reason as given above. This result shows that 442 reactions with no experimental information also have a reasonable quality.

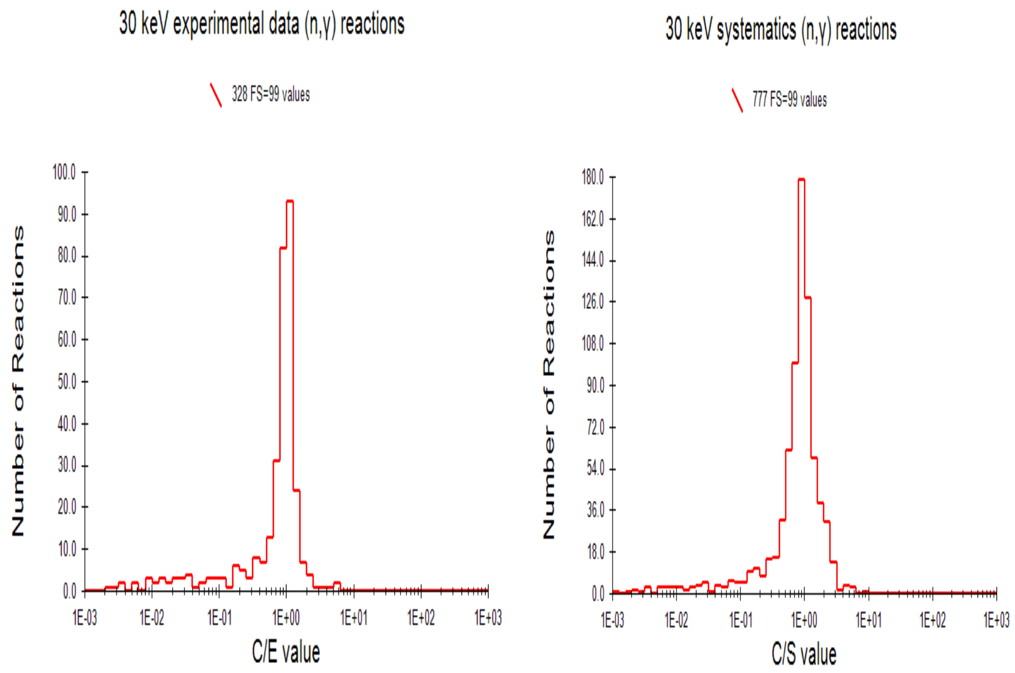

Fig. 6: *C/E histograms of σ(30 keV) against MACS (quasi-monoenergetic) data and systematic predictions.*

4. The possibility to use the C/E values for cross section improvements, is demonstrated in two reactions with strongly deviating C/E values and further discussed in detail in Ref. [4]. The slight underestimation of TENDL-2012 data (trend value 0.94) may be caused by the use of random generation of resolved resonances from average parameters [17].

5. The possibility to increase the accuracy of capture cross sections is rather important to improve the predictive power of theoretical cross section calculations for targets with no experimental support. The MACS validation may play a very important role for this goal as a part of the combined validation with C/E of σ(th), I_γ, MACS and σ(14 MeV). Such validation is able to cover almost completely the excitation curve up to 14 MeV.

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