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# Uncertainty in cross-section calculations for reactions induced by neutrons with energy above 0.1 MeV

*The uncertainty in the calculation of neutron induced reaction cross-sections using modern nuclear models and codes has been investigated. The cross-sections have been calculated with the help of the TALYS code and the modified ALICE code using different models for the calculation of nuclear level density. The experimental data from EXFOR for neutron induced reactions for nuclei from $^{27}$Al to $^{209}$Bi and incident neutron energies above 0.1 MeV have been used for the comparison with calculations. The results obtained give the possibility to find the best approaches for the cross-section calculation for nuclei from different mass ranges.*

***Unsicherheit bei der Berechnung von Wirkungsquerschnitten für Reaktionen induziert durch Neutronen mit einer Energie über 0.1 MeV.*** *Die Unsicherheit bei der Berechnung von Neutronen-induzierten Reaktionsquerschnitten mit Hilfe moderner Kernmodelle und Rechencodes wurde untersucht. Die Wirkungsquerschnitte wurden berechnet mit Hilfe des TALYS Codes und des modifizierten ALICE Codes unter Verwendung verschiedener Modelle zur Berechnung der Kernniveaudichte. Die experimentellen Daten von EXFOR für Neutronen-induzierte Reaktionen bei $^{27}$Al und $^{209}$Bi Kernen und einfallenden Energien von über 0.1 MeV wurden verwendet für den Vergleich mit den Berechnungen. Mit Hilfe der erhaltenen Ergebnisse können die besten Ansätze für die Berechnung von Wirkungsquerschnitten für Kerne verschiedener Massen gefunden werden.*

## 1 Introduction

The evaluation of nuclear reaction cross-sections for neutron threshold reactions is important for a wide number of applications including the activation and transmutation studies for reactors and advanced nuclear units. Usually, the evaluation concerns the analysis of available experimental data and nuclear model calculations.

The present work is devoted to the study of uncertainties in the calculation of activation and transmutation cross-sections for neutron induced reactions. Nuclear models and computer codes having direct relation to the generation of nuclear data files have been selected for calculations. The calculations were performed with the help of nuclear models implemented in the TALYS code [1, 2] and the ALICE/ASH code [3–5], which have been extensively used for nuclear data evaluation [6–13]. The results of calculations are compared with experimental cross-sections from EXFOR for neutron induced reactions for nuclei from $^{27}$Al to $^{209}$Bi.

The deviation factors obtained allow to define appropriate models for nuclear reaction cross-section calculations in different mass ranges of target nuclei.

Methods of calculation are briefly described in Section 2. Evaluated data from nuclear data libraries used for the comparison with calculations and experiments are described in Section 3. The selection of experimental data is discussed in Section 4. The deviation factors used for the comparison of calculations and measured data are discussed in Section 5. Section 6 presents the results of the comparison.

## 2 Brief description of nuclear models used for cross-section calculations

### 2.1 The TALYS code

The pre-equilibrium particle emission is described using the two-component exciton model discussed in Ref. [14]. The model implements new expressions for internal transition rates and new parameterization of the average squared matrix element for the residual interaction obtained using the optical model potential from Ref. [15]. The particle-hole density is calculated taking into account the Pauli correction, the pairing correction and the final depth of nuclear potential well. The depth of the potential well has been parameterized as a function of the projectile energy and the mass of the target separately for incident neutrons and protons to reproduce the influence of surface effects on the first stage of interaction [2]. The multiple pre-equilibrium emission is considered up to arbitrary order of particle escape.

The phenomenological model from Ref. [16] is used for the description of the pre-equilibrium complex particle emission from nuclei.

The contribution of direct processes in inelastic scattering is calculated using the ECIS-97 code integrated in the TALYS code. The coupled channel model or DWBA are selected by TALYS using the available information about nuclear level schemes [2]. The phenomenological model is used to describe giant resonance in inelastic channel.

The equilibrium particle emission is described using the Hauser-Feshbach model [2, 17].

In the present work the nuclear level density for equilibrium states has been calculated using different approaches corresponding to the TALYS input parameter ldmodel equal to 1, 2 or 3. For the first two cases, the level density is obtained by the Fermi gas model with the energy dependent level density parameter, as proposed by *Ignatyuk* and coauthors [18]. The model is combined with the "constant temperature" model, which is used at low excitation energies. The individual parameters of the model are available for about 300 nuclei. The parameter ldmodel = 1 presents the common approach, where the collective enhancement is not described explicitly and included in the nuclear level density parameter. The case ldmodel = 2 refers to the vibrational and rotational enhancement factor calculation discussed in Ref. [2]. For both cases the different systematics for asymptotic value of the nuclear level density parameter and the shell damping parameter are used. The systematics of parameters have been obtained in Ref. [2] from a new analysis of experimental data for neutron resonances.

If the individual experimental nuclear level density parameter is available the shell damping parameter is calculated to provide the coincidence with the energy dependent level density parameter at the neutron separation energy.

The third approach (ldmodel = 3) is based on the results of microscopic calculations performed by Goriely and coauthors [19–21] using the Hartree-Fock-BCS model. The data are taken from RIPL-2 [21] in the tabulated form.

The models used for the nuclear level density calculation are briefly listed in Table 1.

The reaction cross-section has been calculated using the optical potential from Ref. [15].

In general, the calculations were performed using default values of input parameters. The exception was the use of different values of the ldmodel parameter, which is responsible for the method of the nuclear level density calculation. The default value of the bins parameter corresponding to the quality of the emission rates integration was increased up to 100.

### 2.2 The ALICE/ASH code

The ALICE/ASH code [3–5] is a modified and advanced version of the ALICE code originated by M. Blann [22].

The geometry dependent hybrid model (GDH) [5, 22, 23] is used for the description of the pre-equilibrium particle emission from nuclei. Intranuclear transition rates are calculated using the effective cross-section of nucleon-nucleon interactions in nuclear matter. Corrections are made to the GDH approach for the treatment of effects in peripheral nuclear regions [5, 12]. The multiple precompound emission includes the description of the escape for two particles.

*Table 1. The definition of symbols and code options used to perform cross-section calculations*

| Symbols | Model for nuclear level density calculation | Code | Input variable |
|---|---|---|---|
| IST(1) | Fermi gas model with the energy dependent nuclear level density parameter, *a(U)* [18] without explicit description of the collective enhancement[1]. The parameters are defined in Ref. [2] | TALYS | ldmodel = 1 |
| IST-C | Fermi gas model with *a(U)* [18] with explicit description of the rotational and vibrational enhancement[1] | TALYS | ldmodel = 2 |
| G | Microscopic calculations using the HF-BCS approach [21] | TALYS | ldmodel = 3 |
| FG | Fermi gas model with a = A/9[1] | ALICE/ ASH | ldopt = 0 |
| IST(2) | Fermi gas model with the energy dependent nuclear level density parameter, *a(U)* [18][1] | ALICE/ ASH | ldopt = 4 |
| SF | Superfluid nuclear model [28, 29] | ALICE/ ASH | Ldopt = 5 |

[1] at low energy of the excitation the “constant temperature” model is used.

The exciton state density is calculated taking into account pairing corrections, the correction for the Pauli principle and the final depth of the nuclear potential well for the exciton state n = 3. The number of neutrons and protons for initial exciton state is calculated using realistic nucleon-nucleon interaction cross-sections in nucleus [5].

The exciton coalescence model [24, 25] and the knock-out model are used for the description of the pre-equilibrium complex particle emission. The parameters of models are discussed in Refs. [4, 5, 26].

The equilibrium emission of particles is described by the Weisskopf-Ewing model [27] without detail consideration of angular momentum. Three models are used for the calculation of nuclear level density in the present work: the Fermi gas model with the level density parameter a = A/9, the model with the energy dependent *a*-parameter [18] and the generalized superfluid model [28, 29]. In the first two cases, the Fermi gas model is combined with the “constant temperature” model at low excitation energy.

In cross-section calculations using the superfluid model systematics values of parameters were used rather than the individual parameter values. The asymptotic value of nuclear level density parameter obtained using the RIPL data [29] is calculated as follows [30] ■/A = 0.118 $-0.172A^{-1/3}$, which replaces the old systematics of the ■-parameter [28].

To exclude the possible difference in the results of calculations performed by the TALYS code and the ALICE/ASH code caused by different values of total nonelastic cross-sections, the cross-sections calculated by the ALICE/ASH code were normalized on the values of nonelastic cross-sections calculated by the TALYS (ECIS) code.

## 3 Evaluated data

The main goal of the present work is to investigate uncertainties of neutron induced reaction cross-sections calculated using modern theoretical approaches. It is also important to compare the experimental data with evaluated cross-sections from nuclear data files. Such comparison concerns the question on the general quality of different evaluations and on the accuracy one may expect from evaluated data comparing with nuclear model calculations.

In the present work the comparison with experimental data is done for cross-sections from ENDF/B-VI (Release 8), FENDL/A-2.0, JEFF-3.0/A, JENDL-3.2 and JENDL-3.3.

## 4 Experimental data

The comparison of experimental data and calculations was done for nuclei from $^{27}$Al to $^{209}$Bi. This range of nuclides contains important structural and other materials used in reactors, fusion units and ADS. The application of statistical nuclear models for these nuclei is justified.

The experimental data were taken from EXFOR. The data selection criteria concern

i) all target nuclei with atomic number from 13 to 83,
ii) the initial neutron energy above 0.1 MeV,
iii) all (n,xnypz$\alpha$) reactions including the inelastic scattering (n, n′). The data were processed by the X4TOC4 code [31] and presented in the C4 format.

The reaction list of the X4TOC4 code has been extended to include all possible reactions, which are available in EXFOR files.

The following data have been excluded from the consideration:

i) out-dated and superceded measurements,
ii) data for targets, which contain natural mixtures of isotopes;
iii) data for reactions with metastable products,
iv) data averaged for a wide range of neutron incident energies,
v) identical data and
vi) data, which are referred in EXFOR as DATA-MIN or DATA-MAX. The last case required the change in the X4TOC4 code. If two or more data sets correspond to the identical reaction, the equal projectile energy, the same first author, and differ by the year of measurement, only the last measurement is left for the comparison with calculations.

The preliminary comparison with calculations has allowed to recognize a number of errors in the compilation of EXFOR files, which have been reported to the BNL Nuclear Data Center. The data have been corrected after the check of original publications or deleted from the processing.

The (n, γ), (n, np), (n, d) and (n, $^3$He) reactions were excluded from the consideration. The EXFOR data for the (n, np) reaction and the (n, d) reaction were omitted, because the TALYS and ALICE/ASH codes calculate the sum of cross-sections for such reactions. The rather scarce data for the (n, $^3$He) reaction were ignored, because the lack of its theoretical prediction. Data for all other reactions, which are available in EXFOR, were used for the comparison with nuclear model calculations.

As a result, the following experimental data were selected for the comparison with calculations

*The projectile*: neutron
*The projectile energy range*: from 0.1 MeV to maximal energy available (64.4 MeV)
*The target range*: with atomic number Z from 13 to 83
*The reactions available*: (n, n′), (n, p), (n, α), (n, t), (n, 2n), (n, nα), (n, 2p), (n, pα), (n, 2α), (n, 3n), (n, 4n), and other reactions noted in EXFOR as (n, x)
*The total number of experimental points (Z, A, E)*: 17.937
*The number of points with projectile energy above 20 MeV*: 615.

Fig. 1 shows the distribution of the experimental points by the target mass and the energy of the projectile. The sharp peak in the lower figure corresponds to the incident neutron energy at 14–15 MeV. The number of measurements at these energies is about 30 per cent of the total number of experimental points considered.

## 5 Statistical criteria used for the comparison of experimental data and calculations

The following deviation factors [32–35] were used for the comparison of the results of calculations and measured data

$$H = \left( \frac{1}{N} \sum_{i=1}^{N} \left( \frac{\sigma_i^{exp} - \sigma_i^{calc}}{\Delta\sigma_i^{exp}} \right)^2 \right)^{1/2}, \tag{1}$$

$$R = \frac{1}{N} \sum_{i=1}^{N} \frac{\sigma_i^{calc}}{\sigma_i^{exp}}, \tag{2}$$

$$D = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{\sigma_i^{exp} - \sigma_i^{calc}}{\sigma_i^{exp}} \right|, \tag{3}$$

$$F = 10^{\left( \frac{1}{N} \sum_{i=1}^{N} \left[ \log(\sigma_i^{exp}) - \log(\sigma_i^{calc}) \right]^2 \right)^{1/2}}, \tag{4}$$

where $\sigma_i^{exp}$ and $\Delta\sigma_i^{exp}$ are the measured cross-section and its uncertainty, $\sigma_i^{calc}$ is the calculated cross-section, N is the number of experimental points.

The F-factor introduced in Ref. [35], Eq. (4) is useful for the comparison of measurements and calculations at intermediate and high energies of primary particles if experimental data are available for limited number of reaction channels and expected deviations between experimental data and model predictions are rather large [36]. For reactions considered in the present work the H-factor, Eq. (1) is evidently of the most importance.

To estimate the uncertainty in the calculated cross-sections, the authors of Refs. [37, 38] have proposed the covariance matrix, with the contribution accounting for the failure of the model of calculations. The matrix, which defines the "model deficiencies", is constructed using the mean model error δu extracted from the reproduction of experimental data by a given reaction model

$$M_{i,j}^{(def)} = C_{i,j} (\delta u)^2 \sigma_i^{calc}(E_i) \sigma_j^{calc}(E_j) \tag{5}$$

where $E_i$ and $E_j$ are kinetic energies of primary particles, coefficients $C_{i,j}$ are defined in Refs. [37, 38].

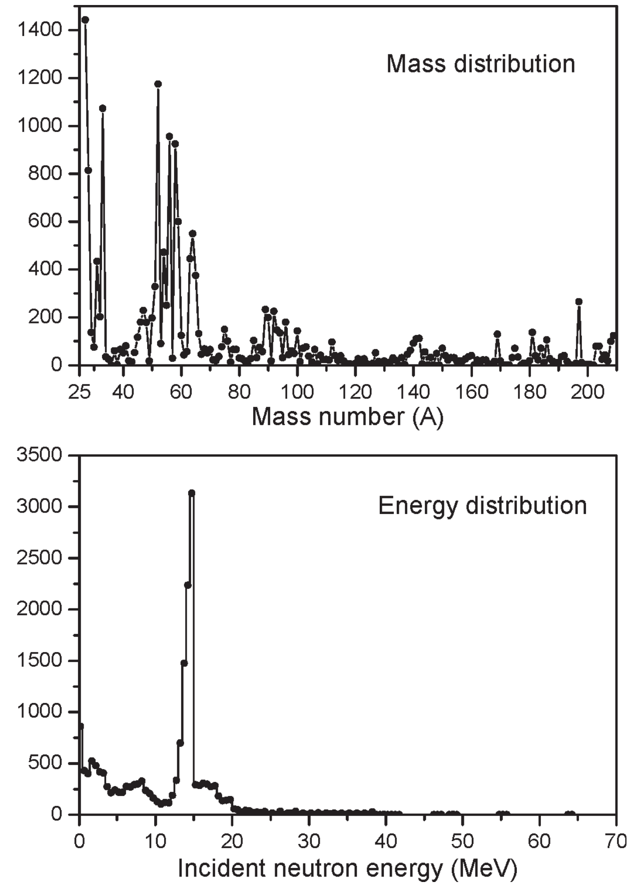

*Fig. 1. The number of experimental points for (n, xnypzα) reaction cross-sections including inelastic neutron scattering (n, n′) available in EXFOR at the neutron incident energy from 0.1 to 64.4 MeV for targets from $^{27}$Al to $^{203}$Bi used for the comparison with calculations, depending upon the mass number of the target nucleus (upper figure) and the projectile energy (lower figure). For the best view points are combined by lines*

The square of the mean model error is used in the present work as an additional factor for estimation of the quality of model calculations

$$L = (\delta u)^2 = \frac{\sum_{i=1}^{N} w_i \left( \frac{\sigma_i^{calc} - \sigma_i^{exp}}{\sigma_i^{calc}} \right)^2}{\sum_{i=1}^{N} w_i} \tag{6}$$

where

$$w_i = \left( \frac{\sigma_i^{calc}}{\Delta\sigma_i^{exp}} \right)^2 \tag{7}$$

The values of deviation factors, Eq. (1)–(4), (6) calculated using different nuclear models and using evaluated cross-sections from nuclear data libraries are discussed below.

## 6 Results and discussion

### 6.1 Comparison of experimental data with nuclear model calculations

#### 6.1.1 General comparison

Table 2 shows the deviation factors, Eq. (1)–(4), (6) calculated for nuclei from $^{27}$Al to $^{209}$Bi without the division into reaction types and target mass regions. The data illustrate the global success or failure of different methods of calculations. The TALYS code shows the best result (the minimal H-value), if the nuclear level density is calculated using the model from Ref. [18] with parameters defined in Ref. [2]. The worst result corresponds to the use of the Fermi gas model with explicit description of the rotational and vibrational enhancement [2].

#### 6.1.2 Medium and heavy nuclei

Table 3 gives the information about the reproduction of experimental data for different mass ranges. Data are subdivided into two ranges by the atomic mass number below and above 120. Approximately, the division corresponds to the dominate contribution of equilibrium (A < 120) and precompound (A > 120) processes in the (n, p) and (n, α) reaction, which give about 58 % of the total number of experimental points.

The use of the TALYS code with the Fermi gas model from Ref. [18] applied for the nuclear level density calculations

*Table 2. Deviation factors for nuclei from $^{27}$Al to $^{209}$Bi calculated using the TALYS and ALICE/ASH codes. The best result is underlined. See Table 1 for symbols explanation*

| Factors | TALYS | | | ALICE/ASH | | |
|---|---|---|---|---|---|---|
| | IST (1) | IST-C | G | FG | IST (2) | SF |
| H | 10.35 | 30.60 | 12.61 | 16.18 | 28.87 | 13.78 |
| R | 1.26 | 1.60 | 1.29 | 1.05 | 0.79 | 1.00 |
| D | 0.50 | 1.05 | 0.57 | 0.53 | 0.64 | 0.52 |
| F | 2.09 | 2.88 | 2.14 | 2.81 | 18.31 | 3.55 |
| L | 0.14 | 0.59 | 0.21 | 0.29 | 0.60 | 0.23 |
| Number of points | 17296 | 17270 | 17295 | 17136 | 17050 | 17122 |

*Table 3. Deviation factors for nuclei with mass number in the ranges 27 = A < 120 and 120 = A = 209 calculated using the TALYS and ALICE/ASH codes. The best result is underlined for each group of nuclei. See Table 1 for symbols explanation*

| Factors | TALYS | | | ALICE/ASH | | |
|---|---|---|---|---|---|---|
| | IST (1) | IST-C | G | FG | IST (2) | SF |
| Targets with atomic mass number 27 = A < 120 | | | | | | |
| H | 10.33 | 29.34 | 12.01 | 17.50 | 31.38 | 14.88 |
| R | 1.25 | 1.57 | 1.27 | 1.06 | 0.78 | 1.01 |
| D | 0.50 | 1.06 | 0.56 | 0.56 | 0.68 | 0.56 |
| F | 2.10 | 2.97 | 2.15 | 2.93 | 22.39 | 3.76 |
| L | 0.13 | 0.55 | 0.18 | 0.29 | 0.60 | 0.24 |
| Number of points | 14467 | 14441 | 14466 | 14313 | 14277 | 14304 |
| 120 = A = 209 | | | | | | |
| H | 10.45 | 36.39 | 15.31 | 6.15 | 7.38 | 5.44 |
| R | 1.32 | 1.77 | 1.38 | 1.03 | 0.84 | 0.95 |
| D | 0.50 | 0.95 | 0.58 | 0.36 | 0.42 | 0.34 |
| F | 2.03 | 2.41 | 2.08 | 2.19 | 4.42 | 2.49 |
| L | 0.27 | 0.77 | 0.44 | 0.14 | 0.29 | 0.13 |
| Number of points | 2829 | 2829 | 2829 | 2823 | 2773 | 2818 |

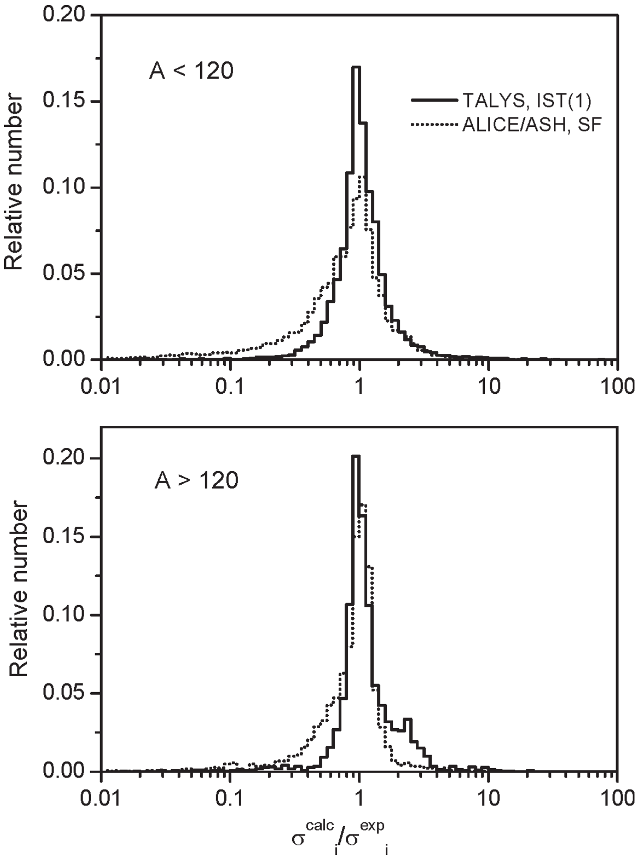

*Fig. 2. The statistics of the ratio of calculated cross-sections to measured cross-sections obtained using results of TALYS code calculations with the help of the Fermi gas model from Ref. [18] and using ALICE/ASH code calculations performed with the help of the superfluid model [28, 29]. For the best view points are combined by histograms*

*Table 4. The H factor for groups of nuclei calculated using the TALYS and ALICE/ASH codes. The best result is underlined for each range of mass number. See Table 1 for symbols explanation*

| Mass Range | TALYS | | | ALICE/ASH | | |
|---|---|---|---|---|---|---|
| | IST (1) | IST-C | G | FG | IST (2) | SF |
| 27 = A < 29 | 8.12 | 18.45 | 14.21 | 9.98 | 14.94 | 10.68 |
| 29 = A < 34 | 14.37 | 12.92 | 13.43 | 31.22 | 91.88 | 23.12 |
| 34 = A < 39 | 4.96 | 11.82 | 4.57 | 5.86 | 5.99 | 6.37 |
| 39 = A < 44 | 5.26 | 19.64 | 6.04 | 17.73 | 13.99 | 17.22 |
| 44 = A < 49 | 13.43 | 9.23 | 11.33 | 18.06 | 20.74 | 11.55 |
| 49 = A < 54 | 11.73 | 18.76 | 12.28 | 12.04 | 13.63 | 13.23 |
| 54 = A < 59 | 10.03 | 14.74 | 10.95 | 20.42 | 20.11 | 14.72 |
| 59 = A < 64 | 11.85 | 49.19 | 16.14 | 26.70 | 15.06 | 23.58 |
| 64 = A < 69 | 8.65 | 22.81 | 11.88 | 7.65 | 18.17 | 7.44 |
| 69 = A < 74 | 7.20 | 97.03 | 10.64 | 11.04 | 16.78 | 19.80 |
| 74 = A < 79 | 5.22 | 33.24 | 5.70 | 3.54 | 5.38 | 4.34 |
| 79 = A < 84 | 5.19 | 15.64 | 5.16 | 6.45 | 7.33 | 6.01 |
| 84 = A < 89 | 4.13 | 14.46 | 4.65 | 4.56 | 6.50 | 4.94 |
| 89 = A < 94 | 10.76 | 51.11 | 9.62 | 15.57 | 17.80 | 11.00 |
| 94 = A < 99 | 5.11 | 47.22 | 6.56 | 6.02 | 6.34 | 6.94 |
| 99 = A < 104 | 8.77 | 41.29 | 8.25 | 7.54 | 6.49 | 21.02 |
| 104 = A < 109 | 4.39 | 20.70 | 3.15 | 5.96 | 5.38 | 6.73 |
| 109 = A < 114 | 7.22 | 31.36 | 10.50 | 8.78 | 7.86 | 12.82 |
| 114 = A < 119 | 21.15 | 38.43 | 19.69 | 21.99 | 20.61 | 21.56 |
| 119 = A < 124 | 9.83 | 11.81 | 10.21 | 3.74 | 4.92 | 4.06 |
| 124 = A < 129 | 9.84 | 14.98 | 13.53 | 5.48 | 14.94 | 10.05 |
| 129 = A < 134 | 8.54 | 50.92 | 9.66 | 5.89 | 7.26 | 7.35 |
| 134 = A < 139 | 4.82 | 28.47 | 4.74 | 6.37 | 9.14 | 7.62 |
| 139 = A < 144 | 9.22 | 18.36 | 10.13 | 4.88 | 5.64 | 4.24 |
| 144 = A < 149 | 5.58 | 7.07 | 5.60 | 4.98 | 7.96 | 5.05 |
| 149 = A < 154 | 7.70 | 8.96 | 7.48 | 6.76 | 8.47 | 5.17 |
| 154 = A < 159 | 5.86 | 4.59 | 4.74 | 4.88 | 8.67 | 4.70 |
| 159 = A < 164 | 10.10 | 10.25 | 9.61 | 4.40 | 5.78 | 3.76 |
| 164 = A < 169 | 13.78 | 18.39 | 13.15 | 4.92 | 6.06 | 5.24 |
| 169 = A < 174 | 4.02 | 4.51 | 4.91 | 6.35 | 8.53 | 5.46 |
| 174 = A < 179 | 5.48 | 6.02 | 5.82 | 4.47 | 6.99 | 4.24 |
| 179 = A < 184 | 17.62 | 18.01 | 17.45 | 3.42 | 6.48 | 3.39 |
| 184 = A < 189 | 5.75 | 8.55 | 5.51 | 3.95 | 5.85 | 4.22 |
| 189 = A < 194 | 4.44 | 4.38 | 4.17 | 7.90 | 3.90 | 3.56 |
| 194 = A < 199 | 16.62 | 24.34 | 16.76 | 5.39 | 7.40 | 4.63 |
| 199 = A < 204 | 8.25 | 6.61 | 12.68 | 16.19 | 7.79 | 8.30 |
| 204 = A = 209 | 10.91 | 88.75 | 31.47 | 7.14 | 7.66 | 7.12 |

shows the best result for A < 120. The ALICE/ASH code has the minimum H-value for the target mass number range A > 120. The best reproduction of experimental data corresponds to the use of the superfluid model for the calculation of the nuclear level density.

Fig. 2 shows the statistics for the calculated and measured cross-sections ratio, σcalc/σexp, obtained using results of the TALYS and ALICE/ASH code calculations. In the first case, the Fermi gas model [18] was used for the nuclear level density calculation. The superfluid model [28, 29] has been applied for the ALICE/ASH code calculations.

### 6.1.3 Various mass ranges

The limited volume of the paper does not allow to present the detailed information about deviation factors calculated for all individual nuclei. As a compromise, the results are shown for H deviation factors for different mass range of target nuclei in the step of ΔA equal to 5.

Table 4 shows the H-factor calculated for various target mass regions. The H- and R-values, which correspond to the TALYS calculations, are shown in Fig. 3. The results obtained using the ALICE/ASH code are presented in Fig. 4. The H- and R-deviation factors calculated using the TALYS and ALICE/ASH codes with the model from Ref. [18] and from Refs. [28, 29], respectively, are shown in Fig. 5.

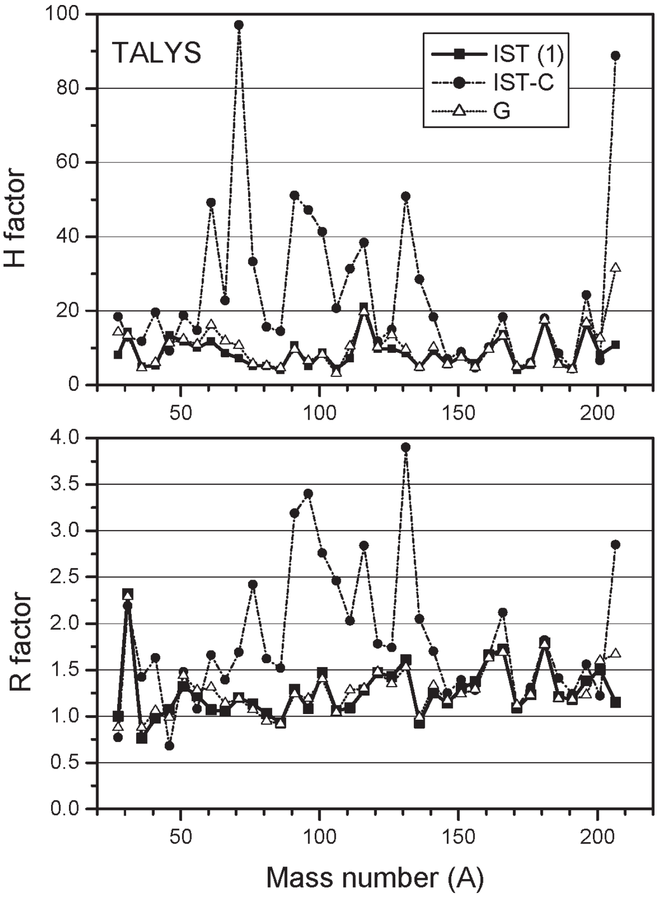

*Fig. 3. The H- and R-deviation factors as functions of the target atomic mass number (A) calculated by the TALYS code using three different models for the nuclear level density calculation (Table 1). Results are relative to the range 27 = A = 209. The first point is calculated averaging the values for target nuclei with mass number in the range 27 = A < 29. All following points represent the average of results relative to target nuclei with atomic mass numbers grouped in step by five, the first step being 29 = A < 34. The last point is averaged in the range 204 = A = 209. Calculated points are linearly interpolated*

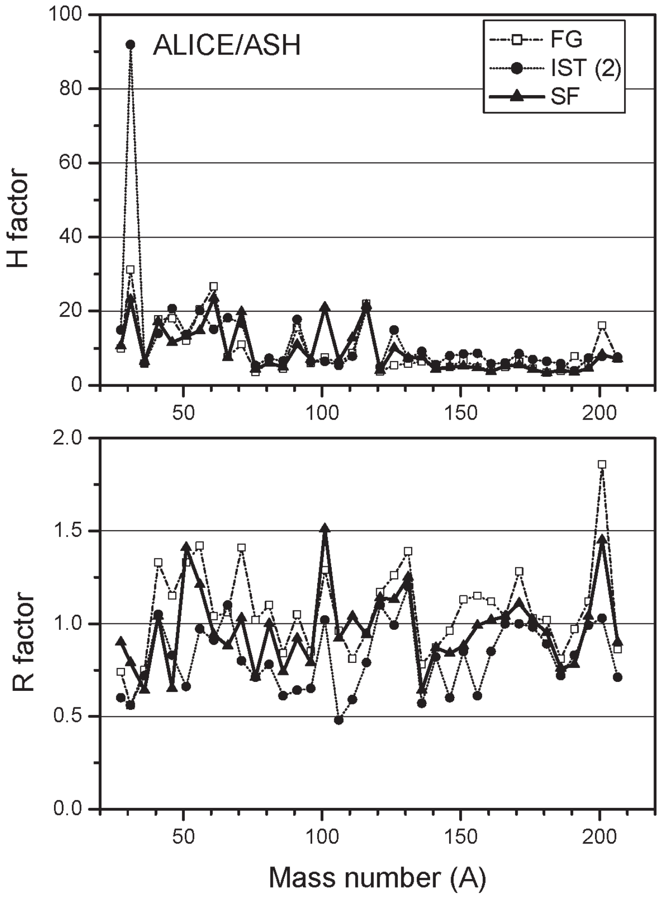

*Fig. 4. The H- and R-deviation factors as functions of the target atomic mass number (A) calculated by the ALICE/ASH code using three different models for the nuclear level density calculation (Table 1). See comments to Fig. 3*

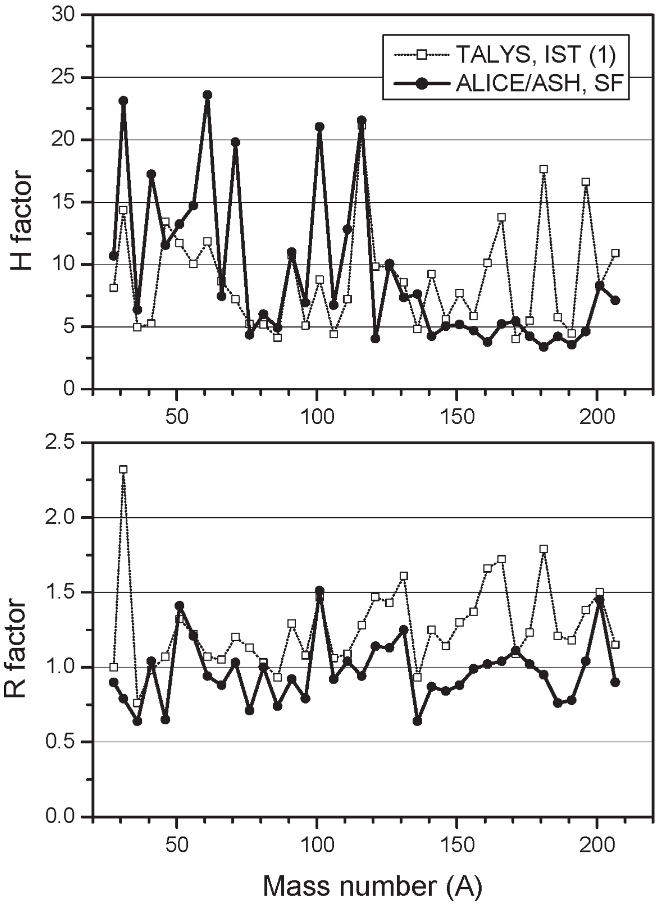

*Fig. 5. The H- and R-deviation factors as functions of the target atomic mass number (A) calculated by the TALYS and ALICE/ASH code. See comments to Fig. 3*

Data presented in Table 4 and in Fig. 5 give the possibility to recommend the use of various nuclear models implemented in the TALYS and ALICE/ASH codes in specific target mass ranges.

### 6.1.4 Individual nuclear reactions

Table 5 shows the value of H-factor, Eq. (1) calculated using the TALYS and ALICE/ASH code for different nuclear reactions in two atomic mass ranges below and above 120.

One can see the success of one or other model in the reproduction of experimental data for individual reactions.

### *6.2 Comparison of experimental data with evaluated data*

The comparison of measured data with evaluations is necessary to answer the question on what the evaluation work adds to the accuracy of the data obtained comparing with calculations using nuclear models.

The deviation factors calculated using data from ENDF/B-VI, FENDL/A-2, JEFF-3/A, JENDL-3.2 and JENDL-3.3 are presented in Table 6. One can see that the data from JEFF-3/A have minimal values of deviations factors comparing with other libraries. The comparison with calculations (Table 3) shows the certain gain in accuracy in the description of experimental data presented by evaluations, at least in the case of the JEFF-3.0/A, ENDF/B-VI and JENDL-3.3 library.

The calculations performed give the possibility to estimate the efficiency of the simple procedure commonly used for the correction of calculated cross-sections. It consists in the renormalization of calculated excitation function using the systematics value at 14.5 MeV. Table 7 shows the results of such correction for the (n, p), (n, α), (n, t) and (n, 2n) reactions. The excitation functions for these reactions calculated by the TALYS and ALICE/ASH codes have been renormalized on cross-section values obtained using semi-empirical systematics at 14.5 MeV from Refs. [39–42]. For the comparison data from JEFF-3/A are presented. Table 7 shows the certain gain in the accuracy of the corrected cross-section for the (n, p) and (n, α) reactions. The renormalization for (n, 2n) and (n, t) reactions seems to be not effective. The results show that the procedure should be used with care and it can not be recommended for reactions with the threshold close to 14.5 MeV, as e. g. for the (n, t) reaction.

## 7 Conclusion

The uncertainty in the calculation of neutron induced reaction cross-sections using modern nuclear models and codes has been studied. The calculation of cross-sections has been performed with the TALYS code [2] and the ALICE/ASH code [5] using different models for the calculation of the nuclear level density (Table 1). The experimental data available in EXFOR for neutron induced reactions for target nuclei from $^{27}$Al to $^{209}$Bi and incident neutron energies above 0.1 MeV have been used for the comparison with calculations. Various deviations factors, Eq. (1)–(4), (6) have been applied for the quantification of the difference between results of calculations and measured data.

*Table 5. The H factor for individual reactions for target nuclei with mass number in the range 27 = A < 120 and 120 = A = 209 calculated using the TALYS and ALICE/ASH codes. The best result is underlined for each reaction. See Table 1 for symbols explanation*

| Reaction | TALYS | | | ALICE/ASH | | |
|---|---|---|---|---|---|---|
| | IST (1) | IST-C | G | FG | IST (2) | SF |
| Targets with atomic mass number 27 = A < 120 | | | | | | |
| (n. n′) | 12.77 | 12.48 | 12.79 | 13.00 | 16.71 | 13.00 |
| (n. 2n) | 13.56 | 14.94 | 13.32 | 31.48 | 60.77 | 22.62 |
| (n. 3n) | 13.35 | 3.04 | 15.27 | 11.62 | 6.24 | 11.67 |
| (n. p) | 8.22 | 28.07 | 9.31 | 10.93 | 19.38 | 12.74 |
| (n. α) | 7.91 | 44.57 | 13.76 | 10.71 | 11.23 | 10.50 |
| (n. t) | 20.52 | 30.62 | 21.04 | 5.12 | 5.70 | 5.09 |
| Others | 7.20 | 4.83 | 7.98 | 9.98 | 15.62 | 10.52 |
| All reactions | 10.33 | 29.34 | 12.01 | 17.50 | 31.38 | 14.88 |
| 120 = A = 209 | | | | | | |
| (n. n′) | 2.17 | 2.62 | 2.22 | 2.11 | 5.68 | 2.52 |
| (n. 2n) | 3.81 | 4.33 | 3.96 | 5.09 | 7.60 | 4.94 |
| (n. 3n) | 4.65 | 4.76 | 5.22 | 12.49 | 10.92 | 5.98 |
| (n. p) | 17.80 | 23.60 | 18.29 | 32.81 | 6.99 | 6.53 |
| (n. α) | 11.56 | 96.20 | 33.74 | 5.45 | 6.64 | 5.66 |
| (n. t) | 41.81 | 103.70 | 42.07 | 4.03 | 4.08 | 4.03 |
| Others | 4.80 | 4.56 | 5.63 | 9.04 | 8.88 | 6.91 |
| All reactions | 10.45 | 36.39 | 15.31 | 6.15 | 7.38 | 5.44 |

*Table 6. Deviation factors for nuclei with mass number in the ranges 27 = A < 120 and 120 = A = 209 calculated using evaluated cross-sections from different nuclear data libraries. The best results are underlined*

| Factors | ENDF/B-VI.8 | FENDL-2/A | JEFF-3/A | JENDL-3.2 | JENDL-3.3 |
|---|---|---|---|---|---|
| Targets with atomic mass number 27 = A < 120 | | | | | |
| H | 8.13 | 76.26 | 7.05 | 24.42 | 8.28 |
| R | 1.09 | 2.17 | 1.23 | 1.83 | 1.69 |
| D | 0.26 | 1.34 | 0.44 | 1.02 | 0.88 |
| F | 1.48 | 2.10 | 1.91 | 2.05 | 2.03 |
| L | 0.06 | 0.87 | 0.06 | 0.43 | 0.08 |
| Number of points | 10 497 | 12 591 | 12 542 | 13 802 | 13 516 |
| 120 = A = 209 | | | | | |
| H | 14.12 | 6.29 | 6.10 | 7.45 | 7.40 |
| R | 1.34 | 1.14 | 1.11 | 1.19 | 1.19 |
| D | 0.54 | 0.33 | 0.26 | 0.38 | 0.38 |
| F | 2.30 | 2.03 | 1.94 | 2.22 | 2.22 |
| L | 0.41 | 0.14 | 0.14 | 0.19 | 0.19 |
| Number of points | 1693 | 2571 | 2548 | 1836 | 1902 |

*Table 7. The deviation factors for various nuclear reactions and target nuclei with atomic mass number 40 ≤ A ≤ 209 obtained using the results of TALYS and ALICE/ASH calculations before and after corrections performed by the 14.5 MeV systematics. See explanations in the text*

| Factor | TALYS | | ALICE/ASH | | JEFF-3/A |
|---|---|---|---|---|---|
| | IST(1) | Corrected | SF | Corrected | |
| (n, p) reaction | | | | | |
| H | 8.89 | 6.05 | 11.23 | 8.29 | 6.40 |
| R | 1.20 | 1.04 | 0.74 | 0.95 | 1.11 |
| D | 0.43 | 0.33 | 0.50 | 0.41 | 0.28 |
| F | 1.80 | 1.66 | 3.85 | 3.26 | 1.72 |
| L | 0.14 | 0.09 | 0.47 | 0.16 | 0.083 |
| Number of points | 4603 | 4603 | 4505 | 4505 | 4538 |
| (n, α) reaction | | | | | |
| H | 7.79 | 5.34 | 10.28 | 5.68 | 6.28 |
| R | 1.14 | 0.98 | 1.03 | 0.88 | 1.08 |
| D | 0.45 | 0.35 | 0.58 | 0.36 | 0.26 |
| F | 1.97 | 1.89 | 2.84 | 2.42 | 1.84 |
| L | 0.21 | 0.126 | 0.29 | 0.16 | 0.15 |
| Number of points | 2159 | 2159 | 2155 | 2155 | 2136 |
| (n, t) reaction | | | | | |
| H | 30.81 | 17.85 | 4.55 | 12.99 | 11.09 |
| R | 3.71 | 2.28 | 0.76 | 2.35 | 1.76 |
| D | 3.05 | 1.79 | 0.73 | 1.76 | 1.11 |
| F | 4.39 | 3.02 | 23.87 | 3.93 | 3.53 |
| L | 0.74 | 0.67 | 0.59 | 0.69 | 0.67 |
| Number of points | 72 | 72 | 78 | 78 | 66 |
| (n, 2n) reaction | | | | | |
| H | 10.54 | 11.53 | 15.85 | 16.90 | 6.88 |
| R | 1.10 | 1.13 | 1.13 | 1.16 | 1.05 |
| D | 0.26 | 0.30 | 0.36 | 0.37 | 0.15 |
| F | 1.46 | 1.50 | 1.65 | 1.62 | 1.29 |
| L | 0.09 | 0.10 | 0.16 | 0.19 | 0.04 |
| Number of points | 4456 | 4456 | 4443 | 4443 | 4164 |

The comparison with experimental data shows that the use of the TALYS code and the Fermi gas model [18] with parameters from Ref. [2] for the calculation of the nuclear level density gives the best description of measured data for target nuclei with A < 120 (Table 3). The ALICE/ASH code and the superfluid model [28, 29] applied for nuclear level density calculation is better for targets with A > 120 (Table 3).

The detailed information about the deviation factors calculated for different groups of nuclei is given in Table 4. The data obtained give the possibility to define the best code and the approach for the nuclear level density calculation for each group of nuclei. The models considered can be recommended for practical calculations of cross-sections for various target mass ranges.

The comparison has been performed also for evaluated cross-sections from nuclear data libraries and experimental data. The results show what gain in the accuracy one should expect from the evaluation work comparing with calculations using nuclear models (Tables 3 and 6).

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