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Notes

Global Comparison of TALYS and ALICE Code Calculations and Evaluated Data from ENDF/B, JENDL, FENDL and JEFF Files with Measured Neutron Induced Reaction Cross-sections at Energies above 0.1 MeV

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The neutron induced reaction cross-sections for target nuclei from ^{27}Al to ^{209}Bi and incident neutron energies above 0.1 MeV have been calculated with the TALYS code and the modified ALICE code using different models for the description of the nuclear level density. Several thousand experimental points from EXFOR have been used for the comparison with these calculations. The obtained results give the possibility to find the best approaches for the cross-section calculation for nuclei in different mass ranges.

Introduction

The goal of the work is the study of uncertainties in the calculation of activation and transmutation cross-sections for neutron induced reactions using nuclear models and codes having direct relation to the generation of nuclear data files. The calculations were performed with the TALYS code[1] and the ALICE/ASH code,[2-4] which have been extensively used for nuclear data evaluation during the last decade.[5-9] The results of calculations are compared with experimental cross-sections from EXFOR[10] for neutron induced reactions for nuclei from ^{27}Al to ^{209}Bi. The comparison is done for main reaction channels, for which experimental data are available, without the distinction. The obtained deviation factors allow to define appropriate models for nuclear reaction cross-section calculation at different mass ranges of target nuclei.

1. Brief description of nuclear models applied for cross-section calculations

1.1. The TALYS code. The pre-equilibrium particle emission is described using the two-component exciton model.[11] 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 Reference 12. The phenomenological model[13] is used for the description of the pre-equilibrium complex particle emission. The contribution of direct processes in inelastic scattering is calculated using the ECIS-97 code incorporated in TALYS.

The equilibrium particle emission is described using the Hauser-Feshbach model. In the present work the nuclear level density for equilibrium states is calculated using different nuclear models,[14,15] which are briefly described in Table 1.

The cross-sections for total neutron nonelastic interactions with nuclei have been calculated using the optical potential from Reference 12.

1.2. The ALICE/ASH code. The ALICE/ASH code[2-4] is a modified and advanced version of the ALICE code.[16]

The geometry dependent hybrid model[17] (GDH) 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 model for the treatment of effects in peripheral nuclear regions.[4,8] The number of neutrons and protons for initial exciton state is calculated using realistic nucleon-nucleon interaction cross-sections in nucleus.[4] The exciton coalescence model[18,19] and the knock-out model are used for the description of the pre-equilibrium complex particle emission.

The equilibrium emission of particles is described by the Weisskopf-Ewing model without detail consideration of angular momentum. Three models,[14,16,20,21] which are briefly described in Table 1, are used for the calculation of nuclear

Table 1: The list of the models used for the calculation of the nuclear level density

Symbols	Model for nuclear level density calculation	Code	Input variable
IST(1)	Fermi gas model with the energy dependent nuclear level density parameter,[14] $a(U)$ without explicit description of the collective enhancement**. The parameters are defined in Reference 1	TALYS	ldmodel=1
IST-C	Fermi gas model[14] with $a(U)$ with explicit description of the rotational and vibrational enhancement**	TALYS	ldmodel=2
G	Microscopic calculations using the HF-BCS approach[15]	TALYS	ldmodel=3
FG	Fermi gas model[16] with $a=A/9$**	ALICE/ASH	ldopt=0
IST(2)	Fermi gas model with the energy dependent nuclear level density parameter,[14,16] $a(U)$**	ALICE/ASH	ldopt=4
SF	Superfluid nuclear model[20,21]	ALICE/ASH	ldopt=5

**At low energy of the excitation the "constant temperature" model is used.

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level density.

To exclude the possible difference in results of calculations performed by codes caused by the use of different values of 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-97) code.

2. Evaluated data

The most complete evaluated data sets were used for the comparison with measured cross-sections. The data were taken from the widely used release of the ENDF/B library (ENDF/B-VI, Release 8),[22] the last version of the library (ENDF/B-VII beta 1),[22] the Fusion Evaluated Nuclear Data Library (Activation Sublibrary, FENDL/A-2.0)[23] and from European Activation File (JEFF-3.0/A).[24] Taking into account the completeness of JENDL-3.2[25] and JENDL-3.3[26] files, both old and new version of the library have been used for the comparison with experimental data.

Such comparison concerns the question on the general quality of different evaluations and on the accuracy one may expect from evaluated data compared with that from nuclear model calculations.

3. Experimental data

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 up to the maximal energy available (64.4 MeV), iii) all (n, $xnypz\alpha$) reactions including the neutron inelastic scattering (n,n').

The data excluded from the consideration are i) out-dated and superceded measurements, ii) measurements for targets, which contain natural mixtures of isotopes, iii) data for reactions with metastable products, iv) identical data, v) data which are referred in EXFOR to DATA-MIN or DATA-MAX, and vi) data for the (n, γ), (n, np), (n, d) and (n, ^{3}He) reactions. Data for (n, np) and (n, d) reactions were omitted, because the TALYS and ALICE/ASH codes calculate the sum of cross-sections for these reactions. The rather scarce data for the (n, ^{3}He) reaction were ignored, because the lack of its theoretical prediction.

As a result, data for the following reactions were selected for the comparison with calculations: (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) used for the comparison is equal to 17,937.

4. Statistical factors used for the comparison of experimental data and calculations

The following deviation factors[27-29] were used for the comparison of the results of calculations and measured data

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

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

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

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

$$L = (\delta u)^2 = \sum_{i=1}^{N} \left(\frac{\sigma_i^{\mathrm{calc}}}{\Delta\sigma_i^{\mathrm{exp}}} \right)^2 \left(\frac{\sigma_i^{\mathrm{calc}} - \sigma_i^{\mathrm{exp}}}{\sigma_i^{\mathrm{calc}}} \right)^2 \Bigg/ \sum_{i=1}^{N} \left(\frac{\sigma_i^{\mathrm{calc}}}{\Delta\sigma_i^{\mathrm{exp}}} \right)^2, \tag{5}$$

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

The use of different factors has been discussed in Reference 30. For the comparison performed in the present work, the H-factor, eq 1, is evidently of the most importance.

Table 2: Deviation factors for nuclei from different mass number ranges calculated using the TALYS and ALICE/ASH codes

Factors	TALYS			ALICE/ASH		
	IST (1)	IST-C	G	FG	IST (2)	SF
Target nuclei with atomic mass number $27 \le A < 120$						
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
$120 \le A \le 209$						
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
All nuclei with $27 \le A \le 209$						
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

The best results are underlined. See Table 1 for symbols explanation.

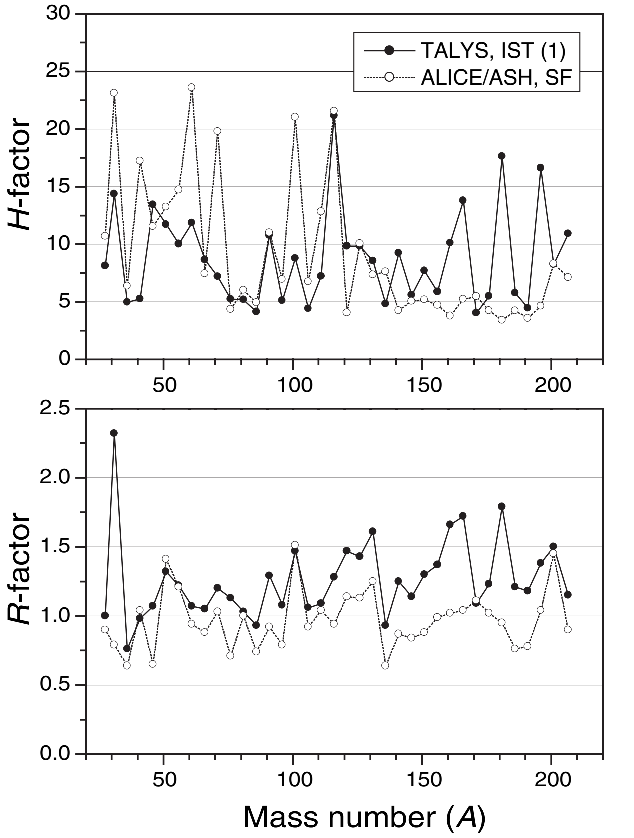

Figure 1. The H- and R-deviation factors, eqs 1 and 2, as functions of the target atomic mass number (A) calculated using the results of the TALYS and ALICE/ASH code calculations. Each point corresponds to the factors calculated at the interval of the mass number ΔA=5. See symbol explanation in Table 1.

5. Results and discussion

Table 2 shows the deviation factors, eqs 1-5, obtained using results of model calculations for nuclei from ^{27}Al to ^{209}Bi. 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 pre-compound (A > 120) processes in the (n, p) and (n, α) reaction, which give about 58% of the total number of experimental points.

The data illustrate the global success or failure of different methods of calculations. The use of the TALYS code with the Fermi gas model[14] applied for the nuclear level density calculations shows the best result for A < 120. The ALICE/ASH code with any input parameters gives a smaller H- value for the target mass number range A > 120 than the TALYS code does. The best reproduction of experimental data is observed with the use of the superfluid model[20,21] for the calculation of the nuclear level density.

Figure 1 shows the H- and R-factors calculated using the TALYS and ALICE/ASH code for various nuclei. Each point on the graph is obtained for the atomic mass range $A_i \pm 2.5$ to improve the statistics. The calculations have been carried out using the Fermi gas model[14] (TALYS) and the superfluid model[20,21] (ALICE/ASH) for the nuclear level density calculation. Data shown in Figure 1 give the possibility to define "the best" nuclear model implemented in TALYS and ALICE/ASH code for specific target mass ranges.

The deviation factors calculated using data from ENDF/B-VI, ENDF/B-VII, FENDL/A-2, JEFF-3/A, JENDL-3.2, and JENDL-3.3 are presented in Table 3. One can see that the data from JEFF-3/A and JENDL-3.3 have smaller values of deviations factors compared with those for other libraries. The comparison with calculations (Table 2) shows the definite advantage of evaluations, at least in the case of JEFF-3.0/A and JENDL-3.3.

6. Conclusion

The global comparison has been done for neutron induced reaction cross-sections calculated using various nuclear models implemented in the TALYS code and the ALICE/ASH code with experimental data from EXFOR. The experimental data for neutron induced reactions for target nuclei from ^{27}Al to ^{209}Bi and incident neutron energies above 0.1 MeV have been

Table 3: Deviation factors for nuclei from different mass number ranges calculated using evaluated cross-sections from different nuclear data libraries

Factors	ENDF/B-VI.8	ENDF/B-VII (beta 1)	FENDL-2/A	JEFF-3/A	JENDL-3.2	JENDL-3.3
Target nuclei with atomic mass number $27 \le A < 120$						
H	8.13	9.56	76.26	7.05	24.42	8.28
R	1.09	1.74	2.17	1.23	1.83	1.69
D	0.26	0.91	1.34	0.44	1.02	0.88
F	1.48	2.02	2.10	1.91	2.05	2.03
L	0.06	0.10	0.87	0.06	0.43	0.08
Number of points	10497	13466	12591	12542	13802	13516
$120 \le A \le 209$						
H	14.12	9.37	6.29	6.10	7.45	7.40
R	1.34	1.20	1.14	1.11	1.19	1.19
D	0.54	0.38	0.33	0.26	0.38	0.38
F	2.30	2.04	2.03	1.94	2.22	2.22
L	0.41	0.27	0.14	0.14	0.19	0.19
Number of points	1693	2257	2571	2548	1836	1902
All nuclei with $120 \le A \le 209$						
H	9.20	9.54	69.54	6.90	23.08	8.18
R	1.12	1.66	2.00	1.21	1.75	1.63
D	0.30	0.83	1.17	0.41	0.95	0.82
F	1.61	2.02	2.09	1.91	2.07	2.06
L	0.09	0.11	0.86	0.06	0.43	0.09
Number of points	12190	15715	15162	15090	15638	15418

The best results are underlined.

selected for the comparison with calculations. The quantification of the difference between results of calculations and measured data has been performed using various deviation factors, eqs 1–5.

The obtained data give the possibility to define the best code and the approach for the nuclear level density calculation for various groups of nuclei. The use of the TALYS code and the Fermi gas model[14] with parameters from in Reference 1 shows the best result for the atomic mass range of target nuclei $A <$ 120. The calculations with the ALICE/ASH code and the superfluid model gives the smallest value of main deviation factors for $A > 120$.

The comparison has been performed for evaluated cross-sections from nuclear data libraries and experimental data. The results show what advantage and accuracy one may expect from the evaluation work compared with model calculations.

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