A. Yu. Konobeyev, C. H. M. Broeders, U. Fischer and L. Mercatali

Uncertainty in activation cross-section calculations at intermediate proton energies

The uncertainty in calculations of proton induced reaction cross-sections using modern nuclear models and codes has been investigated. Cross-sections calculated with TALYS-0.72, ALICE/ASH, DISCA, and MCNPX codes have been compared with experimental data available in EXFOR for (p, x) reactions at proton incident energies up to 150 MeV for target nuclei from ^{24}Mg to ^{209}Bi. In addition, the comparison of evaluated data from ENDF/B-VII, JENDL-HE, and PADF calculations with measured cross-sections has been performed. Various statistical criteria were applied for the quantification of the difference between results of calculations, evaluated and experimental data.

Unsicherheiten bei der Berechnung von Aktivierungsquerschnitten bei mittleren Protonenenergien. Die Unsicherheiten bei der Berechnung protoneninduzierter Wirkungsquerschnitte mit Hilfe moderner Kernmodelle und Rechencodes wurden untersucht. Die Wirkungsquerschnitte wurden mit den Codes TALYS-0.72, ALICE/ASH, DISCA und MCNPX berechnet und mit experimentellen Daten aus EXFOR verglichen. Dabei wurden (p, x)-Reaktionen für Targetkerne von ^{24}Mg bis ^{209}Bi bei Protoneneinfallsenergien bis zu 150 MeV berücksichtigt. Des Weiteren wurden ausgewertete Daten von ENDF/B-VII, JENDL-HE, and PADF mit gemessenen Wirkungsquerschnitten verglichen. Verschiedene statistische Kriterien wurden benutzt, um die Unterschiede zwischen Berechnungen, ausgewerteten und experimentellen Daten zu quantifizieren.

1 Introduction

Recently the uncertainty in activation cross-section calculations performed using different nuclear models at incident nucleon energies up to 150 MeV has been analyzed [1, 2]. The calculation of cross-section has been carried out using the computer codes TALYS-0.64 [3] and ALICE/ASH [4]. Results of the calculation have been compared with available experimental data and evaluated data from JENDL-3.3, JEFF-3/A and ENDF/B-VI.

The release of the new version of the TALYS code implemented by advanced nuclear models [5], ENDF/B-VII [6] and evaluated Proton Activation Data File (PADF) [7] makes it urgent to perform the new comparative analysis of methods of the cross-section calculation and modern evaluated data. It is important to include in the comparison evaluated data from JENDL-HE [10] and results obtained with models and approaches used in the MCNPX code package [8].

The present work is devoted to the analysis of uncertainties in the calculation of activation cross-sections for proton induced reactions. Cross-sections were calculated using different nuclear models and computer codes at proton energies up to 150 MeV. Present analysis supplements the comparison of nuclear models performed recently for the proton energy range from 150 MeV up to 1 GeV [9]. The advantage of evaluated data is demonstrated by the comparison of experimental cross-sections with data from ENDF/B-VI.8, ENDF/B-VII, JENDL-HE, and Proton Activation Data File [7] at energies up to 150 MeV.

2 Activation cross-sections at proton energies up to 150 MeV

2.1 Experimental data

Experimental data used for the comparison with calculations and evaluated data were taken from EXFOR. Measured independent, non-cumulative yields of radionuclides for (p, x) reactions including the radiative capture for target nuclei with the atomic number from 12 to 83 at proton energies from minimal available up to 150 MeV were selected for the comparison.

Following data were excluded from the consideration: i) out-dated, superceded and identical data from EXFOR, ii) measured cross-sections for natural mixtures of isotopes; iii) measured sums of cross-sections for various reactions, iv) data for reactions with meta-stable products, v) experimental data averaged for a wide range of the proton incident energy, vi) approximate data and measured upper and lower limit of cross-sections, and vii) measurements for thick targets.

The preliminary comparison with calculations has shown a number of errors in the compilation of EXFOR files, which have been reported to the NDS, IAEA. Data have been corrected or deleted from the consideration.

As a result, following experimental data were selected for the comparison with calculations
The projectile: protons
The projectile energy range (Ep): from 0 to 150 MeV
Targets: 162 nuclei with atomic number (Z) from 13 to 83 and mass number (A) from 24 to 209
Reactions: 735 proton induced reactions (p, x)
The total number of experimental points (Z, A, Ep): 19, 691. The number of points with proton incident energy below 20 MeV is equal to 9, 370; for Ep from 20 MeV to 50 MeV is equal to 6, 102 and for proton energy from 50 to 150 MeV is equal to 4, 219.

2.2 Deviations factors used for the quantification of the difference between results of calculations and experimental data

Following deviation factors [1, 2, 11, 12] were used for the comparison of results of calculations with experimental data

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

$$D = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{\sigma_i^{exp} - \sigma_i^{calc}}{\sigma_i^{exp}}\right| \quad (2)$$

$$R = \frac{1}{N}\sum_{i=1}^{N}\frac{\sigma_i^{calc}}{\sigma_i^{exp}} \quad (3)$$

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

$$L = \left[\sum_{i=1}^{N}\left(\frac{\sigma_i^{calc}}{\Delta\sigma_i^{exp}}\right)^2\left(\frac{\sigma_i^{calc} - \sigma_i^{exp}}{\sigma_i^{calc}}\right)^2 \Big/ \sum_{i=1}^{N}\left(\frac{\sigma_i^{calc}}{\Delta\sigma_i^{exp}}\right)^2\right]^{1/2} \quad (5)$$

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

In addition, supplementary values [13] were applied to estimate the accuracy of model calculations

$$P1.3 = N1.3/Ntot \quad (6)$$

where N1.3 is the number of points with the ratio $0.77 < \sigma_i^{calc}/\sigma_i^{exp} < 1.33$ and

$$P2.0 = N2.0/Ntot \quad (7)$$

where N2.0 is the number of points with $0.5 < \sigma_i^{calc}/\sigma_i^{exp} < 2.0$, Ntot is the total number of experimental points selected for each type of the comparison.

2.3 Nuclear models and computer codes used for nuclear reaction cross-section calculations

Pre-equilibrium exciton model [14], geometry dependent hybrid model [15], different versions of the intranuclear cascade model [16–18], and various models for the description of nuclear level density [19–23] implemented in popular computer codes were used for the cross-section calculation.

2.3.1 The TALYS code: pre-equilibrium exciton model and Hauser-Feshbach model

The new version of the code [5] has been applied for cross-section calculations.

The pre-equilibrium particle emission is described using the two-component exciton model discussed in Ref. [14]. The contribution of direct processes in the inelastic scattering is calculated using the ECIS-97 code integrated in TALYS. The phenomenological approach from Ref. [24] is applied for the calculation of pre-equilibrium emission rates for complex particles. The equilibrium particle emission is described by the Hauser-Feshbach model [25].

Three models for the calculation of the nuclear level density are compared in the present work

- the Fermi gas model with the energy dependent nuclear level density parameter, as proposed by Ignatyuk and coauthors [19] (IST). The model is combined with the "constant temperature" model, which is used for calculations at low excitation energies [5],
- the "back-shifted" Fermi gas model (BSF) [5, 22],
- the generalized superfluid model (SF) [20, 21].

The reaction cross-section and transmission coefficients have been calculated using the optical potential from Refs. [3, 26].

2.3.2 The ALICE/ASH code: geometry dependent hybrid model and Weisskopf-Ewing model

The ALICE/ASH code [4] is an advanced version of the ALICE code originated by Blann [27].

The geometry dependent hybrid model (GDH) [4, 15, 27] 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. The exciton coalescence model [28, 29] and the knock-out model [30] are used for the description of the pre-equilibrium complex particle emission.

The equilibrium emission of particles is described by the Weisskopf-Ewing model [31] without detail consideration of angular momentum. The nuclear level density is calculated using the generalized superfluid model [20, 21] with different sets of model parameters.

The cross-section for proton nonelastic interactions with nuclei has been calculated using the optical model with parameters from Ref. [26].

2.3.3 The DISCA-C code: advanced intranuclear cascade model and Weisskopf-Ewing model

The code [18] implements the intranuclear cascade evaporation model with the consideration of nucleon-nucleon and nucleon-cluster interactions. The Weisskopf-Ewing model is used for the simulation of the equilibrium emission of neutrons, protons, deuterons, tritons, ^{3}He nuclei and α-particles. The level density for equilibrium states is calculated by the Fermi gas model with the nuclear level density parameter a = A/9 at high excitation energies and by the "constant temperature" model at low energies [27]. Inverse reaction cross-sections are evaluated using phenomenological formulas [32], which approximate results of optical model calculations.

2.3.4 The MCNPX code, Bertini/MPM/Dresner: intranuclear cascade model, pre-equilibrium exciton model and Weisskopf-Ewing model

The default model of the MCNPX code, "Bertini/MPM/Dresner" combines the intranuclear cascade model [16], the pre-equilibrium exciton model [33] and the evaporation model [23]. The nuclear density distribution is approximated by three concentric zones with a constant density [34]. The Multistage Pre-equilibrium Model (MPM) [33] is used for the simulation of the intermediate stage of the nuclear reaction following the intranuclear cascade and preceding the particle evaporation. The nuclear level density is calculated using approximate expressions of the Fermi gas model [34]. The sharp cut-off approximation is used for the evaluation of inverse reaction cross-sections.

2.3.5 The MCNPX code, CEM2k: intranuclear cascade model, pre-equilibrium exciton model and Weisskopf-Ewing model

The Cascade Exciton Model (CEM) model implemented in the MCNPX package was a first model, which combined the advantages of the intranuclear cascade evaporation model and the pre-equilibrium exciton model [35]. The nuclear density distribution is approximated by the step function with seven nuclear regions of the uniform density [34]. Refraction and reflection effects for the nucleon momentum are not considered as in calculations with the Bertini model using the default set of MCNPX input parameters. New approximation for elementary cross-sections is used for the intranuclear event simulation. Many refinements and improvements of the model including the description of momentum-energy conservation on the cascade stage of reactions and new systematics for level density parameters are discussed in Ref. [36].

Cross-sections of (p, x) reactions calculated by all intranuclear cascade evaporation models (DISCA, Bertini/MPM/Dresner, CEM2k) were normalized on proton nonelastic cross-sections, used in ALICE/ASH calculations.

2.4 Evaluated data

Experimental (p, x) reaction cross-sections were compared with data from ENDF/B-VI.8, ENDF/B-VII, JENDL-HE, and PADF at energies from 0 to 150 MeV. PADF contains evaluated data for more than two thousand stable and unstable target nuclei from Mg to Ra at proton incident energies up to 150 MeV, cross-sections were obtained using the TALYS code [3] and the ALICE/ASH code [4]. Results of calculations were corrected using available experimental data from EXFOR.

2.5 Comparison of nuclear model calculations, evaluated and experimental data

2.5.1 Improvement of the agreement between experimental data and calculations performed using new releases of computer codes

Deviation factors, Eq. (1–5) calculated using cross-sections obtained with different versions of the TALYS code: “0.64” [3] and “0.72” [5] are shown in Table 1. Results correspond to the whole mass range of nuclei, investigated in the present work, from 24 to 209, and incident proton energies from 5 to 150 MeV.

Table 2 shows results of the comparison of cross-sections calculated using the ALICE/ASH code and experimental data. The nuclear level density has been calculated using original set [20] and new set [37] of superfluid model parameters.

The better agreement with experimental cross-sections is observed for improved versions of models and codes. At the same time the difference between old and new calculations is rather small (Table 1, 2). Probably, it shows a typical advantage, which one can expect from the successive and gradual improvement of models.

Table 1. Values of deviation factors, Eq.(1)–(5) obtained using (p, x) reaction cross-sections calculated with TALYS-0.64 and TALYS-0.72 for target nuclei from ^{24}Mg to ^{209}Bi at incident proton energies from 5 to 150 MeV. Calculations were performed using different models for the description the nuclear level density for equilibrium states: IST is the Fermi gas model with the energy dependent nuclear level density parameter [5, 19], BSF is the “back-shifted” Fermi gas model [5, 22], SF is the generalized superfluid model [5, 20, 21]. See the text for explanations

Factors	TALYS-0.64	TALYS-0.72		
	IST	IST	BSF	SF
H	22.2	21.1	20.8	21.6
D	0.594	0.576	0.562	0.584
R	1.26	1.230	1.24	1.24
F	2.11	2.15	2.10	2.20
L	0.524	0.490	0.466	0.485
Number of points	162856	16296	16295	16261

Table 2. Values of deviation factors, Eq. (1)–(5) obtained using (p, x) reaction cross-sections calculated with the ALICE/ASH code for target nuclei from ^{24}Mg to ^{209}Bi at incident proton energies from 5 to 150 MeV. Calculations were performed with two set of the SF model parameters [20, 37]. The number of experimental points is equal to 16.068

Factors	ALICE/ASH, SF model	
	Parameters from [20]	Parameters from [37]
H	35.3	26.8
D	0.805	0.719
R	1.42	1.27
F	3.67	3.81
L	0.661	0.598

2.5.2 Description of experimental data at various incident proton energies

Table 3 shows deviation factors and Px values, Eq. (1–7) obtained using results of calculations for target nuclei with atomic numbers from 12 to 83 at the proton energy range from 0 to 150 MeV and between 5 and 150 MeV. Numbers of points shown in the table correspond to non-zero values of cross-sections obtained in each set of calculations.

The best result is observed for the TALYS calculation. Bertini/MPM/Dresner demonstrates the worse agreement with experimental data. Comparison of deviation factors at different proton ranges shows the considerable improvement in the agreement with measured data at the energy range 5–150 MeV. Detailed comparison of H, F, and L-deviation factors at various proton energies is shown in Figs. 1–3 for TALYS and ALICE/ASH codes.

2.5.3 Activation cross-sections for targets with atomic numbers from 21 to 29

Table 4 presents results of the comparison for nuclei with atomic numbers from 21 to 29, which refer to most structural materials proposed for the use in advanced nuclear energy systems.

Calculations with TALYS are considerably better than others. Surprisingly good are results obtained by the Bertini/MPM/Dresner model. Values of deviation factors for Bertini/MPM/Dresner are close to ones obtained with the ALICE/ASH code. Evidently, it results from the fitting of model parameters of Bertini, MPM, and Dresner combination performed in the past for the considered nucleus range.

2.5.4 Activation cross-sections for medium and heavy nuclei

Table 5 shows deviation factors and Px values, obtained using results of model calculations for target nuclei with the atomic number above 40. The ALICE/ASH code has the minimal value of the H-factor and the L factor, which concerns the “model deficiency” [12]. The success is probably related to the GDH model applied for pre-equilibrium particle spectra calculation. Results for Bertini/MPM/Dresner are the same at the proton energy range 0–150 and 5–150 MeV. It is due to lack of calculations at energies 0–5 MeV.

2.5.5 Yields of radionuclides with different mass numbers

The comparison of model calculations of yields of residual nuclei with different masses is presented in Table 6. Data are shown for groups of reaction products with different ΔA equal to the difference of masses for the target and the residual.

One can see that for residual nuclei with ΔA equal to 0 and 1 ALICE/ASH calculations have minimal values of H, R, and L factors. The quality of the description of such reaction is defined by the model used for the simulation on the non-equilibrium particle emission in nuclear reactions. Evidently, data from Table 6 shows the success of the GDH model implemented in the ALICE/ASH code. With the increase of ΔA the agreement between TALYS calculations and experimental data is improved.

Table 3. Values of deviation factors and P1.3, P2.0 values, Eq. (1–7) obtained using (p, x) reaction cross-sections calculated with the help of various codes for target nuclei from ^{24}Mg to ^{209}Bi at different ranges of the incident proton energy. See the text for explanations

Factors	TALYS-0.72 (IST)	TALYS-0.72 (SF)	ALICE/ASH	DISCA-C	Bertini/MPM/Dresner
	Proton energy range from 0 to 150 MeV				
H	122.	121.	543.	620.	2146.
D	1.01	1.10	3.15	4.59	11.1
R	1.69	1.79	3.72	4.95	11.5
F	2.18	2.29	4.75	6.21	6.02
L	0.954	0.946	0.995	0.998	1.00
P1.3	0.455	0.441	0.352	0.247	0.338
P2.0	0.808	0.787	0.661	0.547	0.615
Number of points	19026	18996	18660	17837	15659
	Proton energy range from 5 to 150 MeV				
H	21.1	21.6	26.8	85.1	854.
D	0.576	0.584	0.719	1.39	7.16
R	1.230	1.24	1.27	1.73	7.59
F	2.15	2.20	3.81	4.78	5.91
L	0.490	0.485	0.598	0.943	0.999
P1.3	0.472	0.474	0.390	0.258	0.345
P2.0	0.821	0.815	0.716	0.568	0.620
Number of points	16296	16261	16068	15895	15207

Table 4. Values of deviation factors and P1.3, P2.0 values, Eq. (1)–(7) obtained using (p, x) reaction cross-sections calculated with the help of various codes for target nuclei with the atomic number from 21 to 29 at incident proton energies from 5 to 150 MeV

Factors	TALYS-0.72 (IST)	ALICE/ASH	DISCA-C	CEM2k	Bertini/MPM/Dresner
H	11.8	36.4	144.	467.	34.2
D	0.493	0.926	2.73	2.45	0.83
R	1.12	1.53	3.10	3.00	1.25
F	2.11	2.81	3.85	4.56	3.82
L	0.551	0.840	0.987	0.999	0.949
P1.3	0.486	0.357	0.197	0.268	0.348
P2.0	0.821	0.719	0.520	0.545	0.648
Number of points	5429	5370	5281	4973	5231

2.5.6 Comparison of model calculations, evaluated, and experimental data

ENDF/B-VI.8, ENDF/B-VII and JENDL-HE contain much less information about proton reaction cross-sections than one can find in EXFOR and get from model calculations. For this reason the comparison of codes, evaluated and experimental data was made for (Z, A, Ep) points available in all data sets and calculations. Deviation factors and Px values, Eq. (1–7) are shown in Table 7. In the addition the P10.0 value defined by analogy with Eq. (6, 7) as the relative number of points with the ratio $0.1 < \sigma_i^{calc}/\sigma_i^{exp} < 10$ is given in Table 7.

Results show the improvement in the agreement between measured and evaluated data at the transition from ENDF/B-VI.8 to ENDF/B-VII. JENDL-HE is in the "middle" posi-

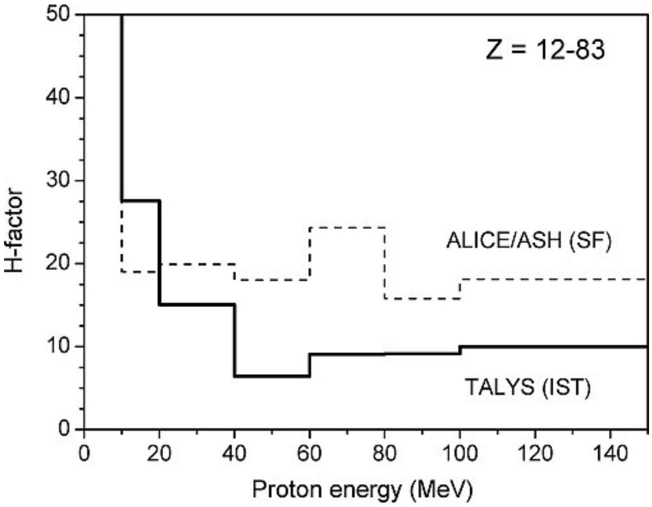

Fig. 1. The value of H-factor, Eq. (1) corresponding to TALYS and ALICE/ASH code calculations for targets with the atomic number from 12 to 83 at various incident proton energy ranges

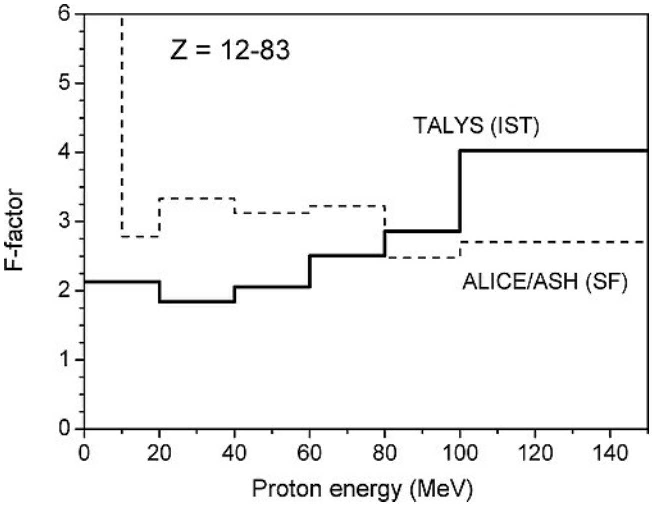

Fig. 2. The same as in Fig. 1, but for the F-deviation factor, Eq. (4)

Table 5. Values of deviation factors and P1.3, P2.0 values, Eq. (1–7) obtained using (p, x) reaction cross-sections calculated with the help of various codes for target nuclei with atomic number from 40 to 83 at different ranges of the incident proton energy

Factors	TALYS-0.72 (IST)	TALYS-0.72 (SF)	ALICE/ASH	DISCA-C	Bertini/MPM/Dresner
	Proton energy range from 0 to 150 MeV				
H	25.8	24.0	20.7	27.1	48.7
D	0.562	0.565	0.641	0.770	0.717
R	1.29	1.28	1.30	1.34	1.31
F	2.14	2.32	3.34	2.86	2.86
L	0.874	0.854	0.812	0.880	0.958
P1.3	0.531	0.527	0.470	0.374	0.442
P2.0	0.837	0.818	0.760	0.709	0.719
Number of points	5333	5332	5263	5101	4377
	Proton energy range from 5 to 150 MeV				
H	24.2	21.9	15.8	22.9	48.7
D	0.542	0.528	0.562	0.702	0.717
R	1.27	1.24	1.23	1.26	1.31
F	2.14	2.33	3.33	2.86	2.86
L	0.867	0.848	0.769	0.872	0.958
P1.3	0.534	0.539	0.482	0.375	0.442
P2.0	0.840	0.823	0.776	0.714	0.719
Number of points	5047	5043	5011	4885	4377

tion, at least for the value of the H-factor. TALYS demonstrates good result comparing with evaluations.

Data from Proton Activation Data File [7] have minimal values of H, R, D, F and L-factors and maximal values of Px.

2.5.7 Agreement between calculations and measurements made in different years

Data in Table 8 answer the question is there the difference in the agreement between predictions of modern nuclear models and experimental data obtained in different years. Calculations were performed by the TALYS code [5] for targets with atomic numbers from 12 to 83 at proton energies from 5 to 150 MeV. One can see a gradual improvement in the agreement between calculations and experimental data obtained since 1980. At the same time deviation factors for old experiments (before 1970) seem surprisingly low.

3 Conclusion

Uncertainties in the calculation of proton induced reaction cross-sections using modern nuclear models and codes have been studied. The calculation of cross-sections has been performed with the help of the TALYS-0.72 code [5], the ALICE/ASH code [4], the DISCA-C code [18], Bertini/

Table 6. Values of H, R, F, and L-deviation factors, and P2.0 values obtained using (p, x) reaction cross-sections calculated with the help of various codes for target nuclei with atomic number from 12 to 83 at the incident proton energy from 5 to 150 MeV for various type of reactions, ΔA = A(target) – A(residual)

Factors	TALYS-0.72 (IST)	ALICE/ASH	DISCA-C	Bertini/MPM/Dresner
	(p, p′) and (p, n) reactions (ΔA = 0)			
H	24.4	23.6	21.0	1383.
R	1.34	1.18	0.887	17.8
F	1.75	3.81	5.68	8.76
L	0.453	0.508	0.525	0.999
P2.0	0.872	0.775	0.627	0.626
Number of points	6018	5988	6032	5788
	Reactions with ΔA = 1			
H	26.6	13.7	26.1	58.5
R	1.23	1.03	0.988	1.39
F	1.99	2.35	4.01	2.42
L	0.519	0.282	0.596	0.762
P2.0	0.858	0.729	0.541	0.780
Number of points	3718	3654	3672	3654
	Reactions with ΔA = 2			
H	14.2	24.2	28.9	45.0
R	1.28	1.58	1.85	2.03
F	2.07	4.03	4.51	2.63
L	0.794	0.888	0.903	0.950
P2.0	0.808	0.641	0.549	0.716
Number of points	1858	1848	1829	1792
	Reactions with ΔA ≥ 3			
H	9.33	20.8	158.	17.1
R	0.991	1.43	3.47	0.924
F	2.80	5.12	4.38	7.53
L	0.681	0.819	0.988	0.918
P2.0	0.730	0.665	0.516	0.420
Number of points	4415	4309	4362	3973

MPM/Dresner and CEM modules from the MCNPX code package [8, 17]. Various approaches were applied for the calculation of the nuclear level density. Results of calculations were compared with experimental cross-sections available in EXFOR for proton induced reactions (p, x) at incident energies from 0 to 150 MeV for target nuclei from 24Mg to 209Bi. Different deviation factors and statistical criteria, Eq. (1–7) have been applied for the quantification of the difference between results of calculations and measured data.

The comparison with experimental data shows that calculations with TALYS provide the best general description of measured cross-sections for the range of target nuclei considered in the present work. The ALICE/ASH code has the minimal value of the H-factor and the "model deficiency" L-factor for target nuclei with atomic number above 40. The good agreement is observed also between DISCA-C calculations and experimental data for targets with $Z \geq 40$.

Evaluated data from ENDF/B-VI.8, ENDF/B-VII, JENDL-HE, and PADF were compared with measured (p, x) reaction cross-sections. The result shows advantages of ENDF/B-VII and PADF data comparing with different kind of calculations. Minimal deviations are observed for PADF.

(Received on 6 August 2007)

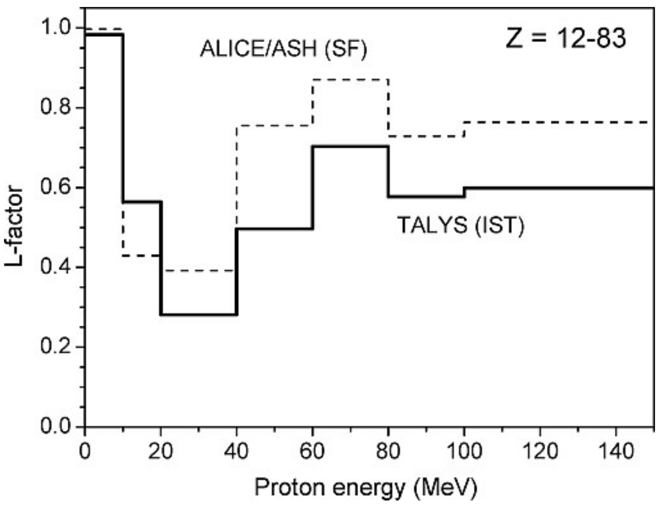

Fig. 3. The same as in Fig. 1, but for the L-factor, Eq. (5)

Table 7. Values of deviation factors and P1.3, P2.0 values, Eq. (1–7) and P10.0 obtained using (p, x) reaction cross-sections calculated with the help of various codes and taken from various data libraries for target nuclei with the atomic number from 12 to 83 at the incident proton energy from 0 to 150 MeV. Number of points is equal to 4125. See explanations in the text

Factors	TALYS-072 (IST)	ALICE/ASH	DISCA-C	Bertini/MPM/Dresner	ENDF/B-VI.8	ENDF/B-VII	JENDL-HE	PADF
H	9.09	16.3	17.2	22.8	9.59	8.14	9.43	4.58
D	0.406	0.643	0.794	0.621	0.450	0.360	0.426	0.118
R	1.10	1.14	1.10	0.886	1.11	1.01	1.14	0.973
F	1.78	3.68	4.62	11.3	1.79	1.74	1.74	1.29
L	0.435	0.699	0.741	0.829	0.513	0.456	0.547	0.285
P1.3	0.500	0.322	0.195	0.314	0.503	0.518	0.505	0.834
P2.0	0.866	0.701	0.554	0.594	0.840	0.857	0.865	0.976
P10.0	0.993	0.938	0.924	0.840	0.992	0.994	0.994	0.999

Table 8. Values of deviation factors and P1.3, P2.0 values, Eq. (1)–(7) obtained using (p, x) reaction cross-sections calculated by TALYS-072 (IST model) and cross-sections measured in different years for nuclei with atomic number from 12 to 83 at proton energy 5–150 MeV

Factors	Years				
	before 1970	1970–1980	1980–1990	1990–1995	after 1995
H	12.6	26.8	30.2	19.7	7.21
D	0.634	0.439	0.806	0.589	0.419
R	1.31	1.14	1.45	1.21	1.03
F	2.10	2.11	2.40	1.92	2.34
L	0.727	0.720	0.339	0.863	0.539
P1.3	0.444	0.538	0.453	0.443	0.485
P2.0	0.774	0.836	0.811	0.857	0.820
Number of points	3448	3514	2749	3980	2605

References

1 *Broeders, C. H. M.; Konobeyev, A. Yu.; Mercatali, L.*: Uncertainty in cross-section calculations for reactions induced by neutrons with energy above 0.1 MeV. Kerntechnik 71 (2006) 174

2 *Broeders, C. H. M.; Konobeyev, A. Yu.; Mercatali, L.*: 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, Journal of Nuclear and Radiochemical Sciences, 7 (2006) N1

3 *Koning, A. J.; Hilaire, S.; Duijvestijn, M. C.*: TALYS-0.64. A nuclear reaction program. User manual. NRG Report 21297/04.62741/P FAI/AK/AK, Dec 5, 2004

4 *Broeders, C. H. M.; Konobeyev, A. Yu.; Korovin, Yu. A.; Lunev, V. P.; Blann, M.*: ALICE/ASH – pre-compound and evaporation model code system for calculation of excitation functions, energy and angular distributions of emitted particles in nuclear reactions at intermediate energies. FZK 7183, 2006; http://bibliothek.fzk.de/zb/berichte/FZKA7183.pdf

5 *Koning, A. J.; Hilaire, S.; Duijvestijn, M. C.*: TALYS-0.72. A nuclear reaction program. User manual. Dec 21, 2006; http://www.talys.eu/the-talys-team/arjan-koning/

6 *Obložinský, P.*: Recent Advances in the ENDF/B Library, Proc. Int. Conf. on Nuclear Data for Science and Technology, Santa Fe, New Mexico, USA, September 26–October 1, 2004, p. 165; http://www.nndc.bnl.gov/exfor4/endf00.htm

7 *Broeders, C. H. M.; Fischer, U.; Konobeyev, A. Yu.; Mercatali, L.; Simakov, S. P.*: "Proton Activation Data File" to Study Activation and Transmutation of Materials Irradiated with Protons at Energies up to 150 MeV, J. Nucl Sci. Technol. (2007), to be published

8 *Hendricks, J. S.; McKinney, G. W.; Durkee, J. W.; Finch, J. P.; Fensin, M. L.; James, M. R.; Johns, R. C.; Pelowitz, D. B.; Waters, L. S.*: MCNPX, Version 26C, LA-UR-06-7991 Dec.7, 2006

9 *Korovin, Yu.; Fischer, U.; Konobeyev, A.; Natalenko, A.; Pilnov, G.; Stankovskiy, A.; Tikhonenko, A.*: Evaluation of activation nuclear data in the energy region from 150 MeV to 1 GeV, Proc. Int. Conf. on Nuclear Data for Science and Technology, Nice, France, April 22–27, 2007

10 *Watanabe, Y.; Fukahori, T.; Kosako, K.; Shigyo, N.; Murata, T.; Yamano, N.; Hino, T.; Maki, K.; Nakashima, H.; Odano, N.; Chiba, S.*: Nuclear Data Evaluations for JENDL High-Energy File, Proc. Int. Conf. on Nuclear Data for Science and Technology, Santa Fe, New Mexico, USA, September 26–October 1 2004, p. 326; http://wwwndc.tokai-sc.jaea.go.jp/ftpnd/jendl/ jendl-he-2004.html

11 *Michel, R.; Bodemann, R.; Busemann, H.; Daunke, R.; Gloris, M.; Lange, H.-J.; Klug, B.; Krins, A.; Leya, I.; Lüpke, M.; Neumann, S.; Reinhardt, H.; Schnatz-Büttgen, M.; Herpers, U.; Schiekel, Th.; Sudbrock, F.; Holmqvist, B.; Condé, H.; Malmborg, H.; Suter, M.; Dittrich-Hannen, B.; Kubik, P.-W.; Synal, H.-A.; Filges, D.*: Cross sections for the production of residual nuclides by low- and medium-energy protons from the target elements C, N, O, Mg, Al, Si, Ca, Ti, V, Mn, Fe, Co, Ni, Cu, Sr, Y, Zr, Nb, Ba and Au. Nucl. Instr. Meth. B129 (1997) 153

12 *Leeb, H.; Pigni, M. T.; Raskinyte, I.*: Covariances for Evaluations based on Extensive Modelling. Proc. Int. Conf. on Nuclear Data for Science and Technology, Santa Fe, USA, Sep. 26–Oct. 1, 2004, p. 161

13 *Titarenko, Yu. E.* (Project manager): Experimental and Theoretical Study of the Yields of Residual Product Nuclei Produced in Thin Targets Irradiated by 100–2600 MeV Protons, ISTC 839B-99, 2001

14 *Koning, A. J.; Duijvestijn, M. C.*: A global pre-equilibrium analysis from 7 to 200 MeV based on the optical model potential. Nucl. Phys. A744 (2004) 15

15 *Blann, M.; Vonach, H. K.*: Global test of modified precompound decay models. Phys. Rev. C 28 (1983) 1475

16 *Bertini, H. W.*: Intranuclear-cascade calculation of the secondary nucleon spectra from nucleon-nucleus interactions in the energy range 340 to 2900 MeV and comparisons with experiment. Phys. Rev. 188 (1969) 1711

17 *Mashnik, S. G.; Sierk, A. J.; Bersillon, O.; Gabriel, T.*: Cascade-exciton model analysis of proton induced reactions from 10 MeV to 5 GeV. Nucl. Instr. Meth. A 414 (1998) 68; LA-UR-97–2905, Los Alamos National Laboratory (1997); http://t2.lanl.gov/publications/publications.html

18 *Broeders, C. H. M.; Konobeyev, A. Yu.; Korovin, Yu. A.; Sosnin, V. N.*: DISCA – advanced intranuclear cascade cluster evaporation model code system for calculation of particle distributions and cross-sections at intermediate energies, FZK 7221, June 2006, http://bibliothek.fzk.de/zb/berichte/FZKA7221.pdf

19 *Ignatyuk, A. V.; Smirenkin, G. N.; Tishin, A. S.*: Phenomenological description of the energy dependence of the level density parameter. Sov. J. Nucl. Phys. 21 (1975) 255

20 *Ignatyuk, A. V.; Istekov, K. K.; Smirenkin, G. N.*: Role of collective effects in the systematics of nuclear level densities. Sov. J. Nucl. Phys. 29 (1979) 450

21 *Ignatyuk, A. V.; Capote, R.*: Nuclear Level Densities, In: Handbook for Calculations of Nuclear Reaction Data, RIPL-2, IAEA-TECDOC-1506 (2006) p. 85, http://www-nds.iaea.org/RIPL-2/handbook.html

22 *Dilg, W.; Schantl, W.; Vonach, H.; Uhl, M.*: Level density parameters for the back-shifted fermi gas model in the mass range $40 < A < 250$ Nucl. Phys. A 217 (1973) 269

23 *Dresner, L.*: EVAP – A Fortran Program for Calculating the Evaporation of Various Particles from Excited Compound Nuclei, Report ORNL-TM-196 (1961)

24 *Kalbach Walker, C. K.*: PRECO-2000: Exciton model preequilibrium code with direct reactions, March 2001; http://www.nndc.bnl.gov/nndcscr/model-codes/preco-2000/index.html

25 *Hauser, W.; Feshbach, H.*: The inelastic scattering of neutrons. Phys. Rev. 87 (1952) 366

26 *Koning, A. J.; Delaroche, J. P.*: Local and global nucleon optical models from 1 keV to 200 MeV. Nucl. Phys. A 713 (2003) 231

27 *Blann, M.*: ALICE-91: Statistical model code system with fission competition. RSIC CODE PACKAGE PSR-146

28 *Iwamoto, A.; Harada, K.*: Mechanism of cluster emission in nucleon-induced preequilibrium reactions. Phys. Rev. C 26 (1982) 1821

29 *Sato, K.; Iwamoto, A.; Harada, K.*: Pre-equilibrium emission of light composite particles in the framework of the exciton model. Phys. Rev. C 28 (1983) 1527

30 *Konobeyev, A. Yu.; Lunev, V. P.; Shubin, Yu. N.*: Pre-equilibrium emission of clusters. Acta Physica Slovaca 45 (1995) 705

31 *Weisskopf, V. F.; Ewing, D. H.*: On the yield of nuclear reactions with heavy elements. Phys. Rev. 57 (1940) 472

32 *Chatterjee, A.; Murthy, K. H. N.; Gupta, S. K.*: Optical reaction cross sections for light projectiles. INDC(IND)-27/GJ, International Atomic Energy Agency (1980)

33 *Prael, R. E.; Bozoian, M.*: Adaptation of the multistage pre-equilibrium model for the monte carlo method (I). LA-UR-88-3238, Los Alamos National Laboratory (Sept. 1988); http://www-xdiv.lanl.gov/XCI/ PEOPLE/rep/plist.html

34 *Waters, L. S.* (editor): MCNPXTM User's manual. Version 2.3.0. LA-UR-02-2607, Los Alamos National Laboratory (2002)

35 *Gudima, K. K.; Mashnik, S. G.; Toneev, V. D.*: Cascade-exciton model of nuclear reactions. Nucl. Phys. A 401 (1983) 329

36 *Mashnik, S. G.; Gudima, K. K.; Moskalenko, I. V.; Prael, R. E.; Sierk, A. J.*: CEM2K and LAQGSM Codes as Event Generators for Space-Radiation-Shielding and Cosmic-Ray-Propagation Applications. Advances in Space Research 34 (2004) 1288

37 *Ignatyuk, A. V.*: Level densities. In: Handbook for Calculations of Nuclear Reaction Data. IAEA-TECDOC-1034. International Atomic Energy Agency Report (1998), p. 65

The authors of this contribution

A. Yu. Konobeyev, C. H. M. Broeders, U. Fischer and *L. Mercatali*, Institut für Reaktorsicherheit, Forschungszentrum Karlsruhe GmbH, 76021, Karlsruhe, Germany

* Corresponding author. E-mail: mercatali@irs.fzk.de.
Tel.: +49 7247 82 2751