AN EXTENSIVE ASSESSMENT OF THE PREDICTIVE CAPABILITIES OF DIFFERENT NUCLEAR MODELS FOR THE CALCULATION OF PROTON INDUCED REACTION CROSS-SECTIONS UP TO 150 MEV

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Abstract

The predictive capabilities of different nuclear models and codes for the calculation of proton induced reaction cross-sections have been investigated. The analysis is relative to the energy range 0.1÷150 MeV and to a large mass number range (24<A<209) relevant for ADS applications. Experimental EXFOR data have been processed and treated in order to systematically analyze all the available measurements relative to proton induced reactions. The comparison between calculations and measurements is performed by means of statistical deviation factors which can be used to provide recommendations on the best combinations of codes and models to optimize the accuracy of the simulations. Furthermore, a mean model parameter has been calculated for selected numbers of experiments, making the results of this work also useful for the construction of covariances matrixes of "model deficiencies" for a wide number of nuclides and popular nuclear models.

Introduction

Accelerator Driven Subcritical Systems (ADS's) are being studied since more than a decade within the framework of the R&D activities related to the P&T strategies. The majority of the ADS designs conceived up to know rely on a proton accelerator to provide via spallation reactions the external neutron source necessary to control the reactivity of the system. Good quality proton cross section data are therefore required to provide a reliable design of such systems. The main purpose of this paper is to provide preliminary results related to the investigation of the uncertainty associated to the calculation of activation and transmutation cross-sections for proton induced reactions using nuclear models and codes.

The TALYS and ALICE/ASH codes

In this work all the calculations have been performed by means of the TALYS code and the ALICE/ASH code [1-2]. The investigation of the performance of these simulation tools is motivated by their extensive use within the international community for the generation of nuclear data files. As far as the TALYS code, the pre-equilibrium particle emission is described using the two-component exciton model [3]. The model implements new expressions for internal transition rates and new parametrization of the average square matrix element for the residual interaction obtained using the optical model potential of Koning et el. [4]. The phenomenological model is used for the description of the pre-equilibrium complex particle emission [5]. The contribution of direct processes in inelastic scattering is calculated using the ECIS-97 code incorporated in TALYS. The equilibrium particle emission is described by means of the Hauser-Feshbach model.

The ALICE/ASH code is a modified and advanced version of the ALICE code [6]. The geometry dependent hybrid model (GDH) is used in the description of the pre-equilibrium particle emission from nuclei [7]. Intranuclear transition rates are calculated using the effective cross-section of nucleon-nucleon interactions in the nuclear matter. The number of neutrons and protons for initial exciton states is calculated using realistic nucleon-nucleon interaction cross-sections in nucleus. The exciton coalescence model and the knock-out model are used for the description of the pre-equilibrium complex particle emission [8]. The equilibrium emission of particles is described by the Weisskopf-Ewing model without detailed consideration of angular momentum.

The calculation of nuclear level densities

For the purposes of the present work, both the TALYS and the ALICE/ASH codes have been used with default values of input parameters, with the exception of the parameters describing the particular model used for the nuclear level densities description. In particular, six different level density models have been considered, corresponding to the input parameters *ldmodel* equal to 1, 2 or 3 and *ldopt* equal to 0, 4 and 5 in the TALYS code and in the ALICE/ASH code respectively. Detailed information on these models can be found in [9-13]. The main features can be summarized as follows:

a. *ldmodel*1: Fermi gas model with the energy dependent level density parameter *a(U)* without explicit description of the collective enhancement.
b. *ldmodel*2: Fermi gas model with the energy dependent level density parameter *a(U)* with explicit description of the rotational and vibrational enhancement.
c. *ldmodel*3: Microscopic model based on the results of microscopic calculations performed by Goriely et al. using the Hartree-Fock-BCS model.
d. *ldopt*0: Fermi gas model with the dependent level density parameter $a=A/9$.

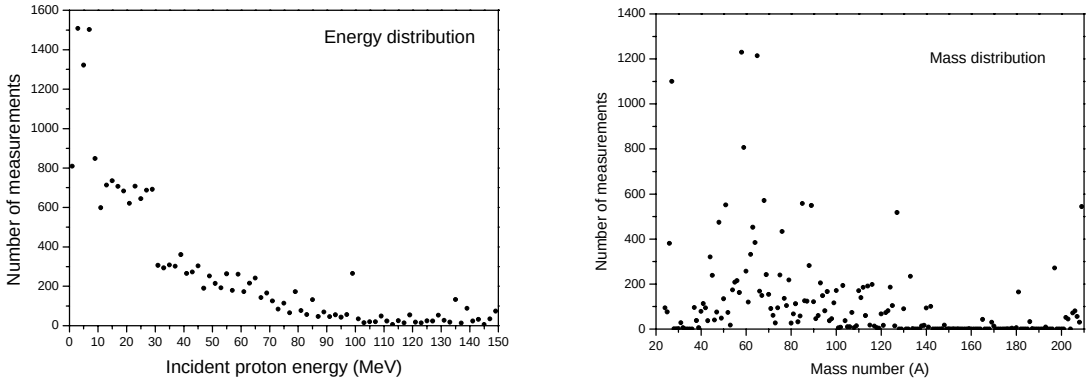
e. *ldopt*4: Fermi gas model with the energy dependent level density parameter *a(U)*.
f. *ldopt*5: Superfluid nuclear model.

In the following we will refer to the results of the calculations performed with the different models with the following notation: *ldmodel*1=IST1, *ldmodel*2=IST-C, *ldmodel*3=G, *ldopt*0=FG, *ldopt*4=IST2, *ldopt*5=SF.

Experimental data and statistical criteria of comparison

The comparison of experimental data and calculations has been performed for nuclei from ^{24}Mg to ^{209}Bi. The experimental data were taken from EXFOR. Independent (non-cumulative) yields of radionuclides in (p,γ), (p,n) and other (p,xnypzα) reactions for target nuclei with atomic number from 12 to 83 in the energy range 0÷150 MeV were selected for the comparison. 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 proton incident energies, v) identical data and vi) data, which are referred in EXFOR as DATA-MIN or DATA-MAX. The total number of experimental points (*Z*,*A*,*E*) used for the comparison is in the order of 19,000. The mass distribution and the energy distribution of the experimental data are shown in Fig. 1.

Fig.1. Distributions of the experimental points



The following statistical factors have been used to quantify the deviation of the calculated results from the measured data:

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

$$R = \frac{1}{N}\sum_{i=1}^{N}\frac{\sigma_i^{calc}}{\sigma_i^{exp}} \quad (2)$$

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

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

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.

To estimate the uncertainty in the calculated cross-sections a covariance matrix has been proposed, which takes into account the contribution to the uncertainty due to the failure of the model used for the calculations [15]. The square of the mean model error is used in the present work as an additional factor to estimate the quality of model calculations, as follows:

$$L = (\delta u)^2 = \frac{\sum_{i=1}^{N} w_i \left(\frac{\sigma_i^{calc} - \sigma_i^{exp}}{\sigma_i^{calc}}\right)^2}{\sum_{i=1}^{N} w_i} \quad (5)$$

where:

$$w_i = \left(\frac{\sigma_i^{calc}}{\Delta\sigma_i^{exp}}\right)^2 \quad (6)$$

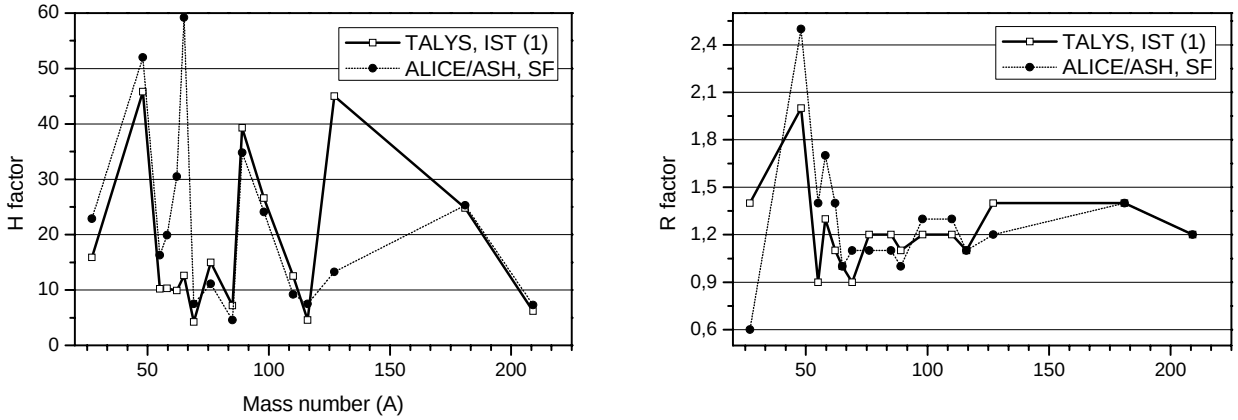
Results

Deviation factors calculated for target nuclei from ^{24}Mg to ^{209}Bi over the entire energy range (0÷150 MeV) and without distinction into reaction types are summarized in Table 1. Results are provided over the entire mass range and in the two atomic mass ranges below and above 120. From the results one can observe that the TALYS code is globally performing better with respect to the ALICE code, particularly in the mass range below 120. The best results are obtained when using the Fermi gas model without the explicit description of the collective enhancement (IST(1) model) and the microscopic model of Goriely (G model). For target nuclei with mass numbers above 120 the ALICE/ASH calculations using the superfluid model (SF) for the nuclear level density determination provide the best results. In Fig. 1 the best performing model of TALYS (IST (1)) is compared with the best one of ALICE/ASH (SF) in the case of the treatment for different mass number ranges.

Table 1. 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 $24 \leq A < 120$						
R	1.76	2.03	1.80	4.97	13.90	4.16
D	1.08	1.42	1.07	4.34	13.44	3.58
F	2.08	2.54	2.07	3.35	14.23	4.80
L	0.91	0.93	0.91	1.00	0.99	0.99
H	22.0	111.6	20.7	851.6	1100.6	625.2
Number of points	16306	16269	16314	16030	15960	15995
$120 \leq A \leq 209$						
R	1.43	1.55	1.67	1.30	1.51	1.21
D	0.69	0.88	0.95	0.75	0.91	0.63
F	2.25	2.98	2.89	4.37	6.16	4.34
L	0.91	0.93	0.91	1.00	0.99	0.99
H	34.2	34.5	41.5	35.0	23.5	16.2
Number of points	2928	2927	2928	2907	2885	2905
All nuclei with $24 \leq A \leq 209$						
R	1.71	1.96	1.78	4.40	12.00	3.71
D	1.02	1.34	1.05	3.79	11.52	3.13
F	2.11	2.61	2.20	3.51	12.74	4.73
L	0.91	0.93	0.91	1.00	0.99	0.99
H	24.4	103.0	25.3	778.4	1006.1	571.4
Number of points	19234	19196	19242	18937	18845	18900

Fig. 2. The H and R deviation factors as functions of different groups of target nuclei mass numbers (A) calculated using the TALYS and ALICE/ASH code



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