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An Extensive Assessment of the Predictive Capabilities of Different Nuclear Models for the Calculation of Proton Induced Reaction Cross-Sections up to 150 MeV

I 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 modern theoretical approach.

II THEORETICAL CALCULATIONS

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. 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. The main features of these models 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.

III EXPERIMENTAL DATA

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 19,253. The mass distribution and the energy distribution of the experimental data are shown in Fig. 1.

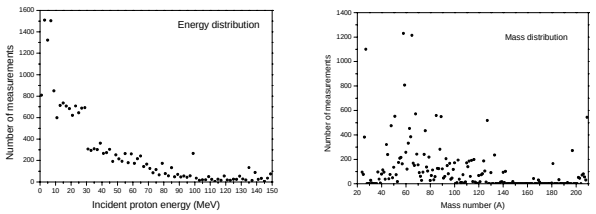

Fig. 1: Distributions of the experimental points

IV STATISTICAL TREATMENT

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

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

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

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

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

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 [3], which takes into account the contribution to the uncertainty due to the failure of the model used for the calculations. The matrix, which defines the "model deficiencies", is constructed using a mean model error δu extracted from the reproduction of experimental data by a given reaction model 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:

$$L = (\delta u)^2 = \frac{\sum_{k=1}^{K} w_k (\delta u_k)^2}{\sum_{k=1}^{K} w_k}$$

where:

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

V 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. 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. 2 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.

Tab. 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
Exp. 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
Exp. 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
Exp. Points	19234	19196	19242	18937	18845	18900

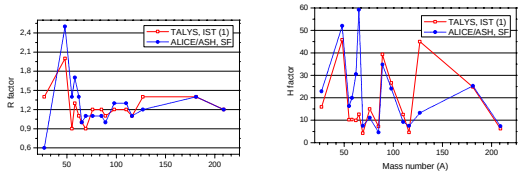

Fig. 2: The H and R deviation factors as functions of different groups of target nuclei mass numbers (A) calculated using the TALYS and ALICE/ASH code

VI REFERENCES

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