IMPLEMENTATION OF THE GEOMETRY DEPENDENT HYBRID MODEL IN TALYS

A.YU. KONOBEYEV*, U. FISCHER, A.J. KONING[1], P.E. PERESLAVTSEV, and M. BLANN[2]
Institut für Neutronenphysik und Reaktortechnik, Karlsruher Institut für Technologie, Postfach 3640, 76021 Karlsruhe, Germany
[1]Nuclear Research and Consultancy Group NRG, Westerduinweg 3, P.O. Box 25, NL-1755 ZG Petten, The Netherlands
[2]75-5865 Walua Rd. D423, Kailua-Kona, Hi. 96740
*Corresponding author. E-mail : konobeev@inr.fzk.de

Received
Accepted for Publication

The geometry dependent hybrid model (GDH) developed by M.Blann and supplied by the models for the non-equilibrium cluster emission was implemented in the TALYS code. A number of subroutines from the ALICE and ALICE/ASH codes were introduced in TALYS after appropriate modifications. Common computations as those relating to binding energies, the optical model and others are performed by means of TALYS. The value of the TALYS input variable "preeqmode" equal to 5 is reserved for the use of the GDH approach for the calculation of the pre-compound energy distributions of nucleon and light clusters. A comparison with calculations using the original ALICE and ALICE/ASH codes, on one hand, and experimental data, on the other hand, is given. The advantages of the implementation of the GDH model in the TALYS code are discussed.

KEYWORDS : nuclear model, geometry dependent model, Hauser-Feshbach model

1. INTRODUCTION

Nearly forty years the geometry dependent hybrid model (GDH) proposed by M.Blann [1] is used successfully for the modelling of non-equilibrium particle and light cluster emission in nuclear reactions induced by intermediate energy particles. A popular application of GDH is associated with Weisskopf-Ewing model, though the advance of the combination with the Hauser-Feshbach model was obviously demonstrated [2].

The TALYS code [3] belongs to the new generation of nuclear model codes combining the wide spectrum of well justified nuclear models and approaches for the simulation of non-equilibrium and equilibrium processes in nuclear reactions. In practice the use of various methods of calculations available by user's choice gives a good possibility to understand their strong and weak points and to obtain the real uncertainty of theoretical predictions of calculated cross-sections and particle distributions in nuclear reactions.

The aim of the present work is to extend the number of nuclear models integrated in TALYS by the implementation of the GDH model and to benefit from the combination of GDH with the Hauser-Feshbach model.

A brief description of implemented models, changes in TALYS, as the comparison with experimental data are given below.

2. BRIEF DESCRIPTION OF MODELS IMPLEMENTED IN TALYS IN THE PRESENT WORK

A new module providing calculations of pre-equilibrium nucleon and light cluster distributions using GDH was added to TALYS. The module consists of a number of subroutines from ALICE/ASH code [4] modified for appropriate integration in TALYS and subroutines written to provide the proper interface between TALYS and modified ALICE/ASH modules.

In the GDH model the pre-equilibrium energy distribution of nucleons is calculated as follows

$$\frac{d\sigma}{d\varepsilon_x} = \pi \bar{\lambda}^2 \sum_{l=0}^{\infty} (2l+1) T_l \times \sum_{n=n_0} {}_nX_x \frac{\omega(p-1,h,U)}{\omega(p,h,E)} \frac{\lambda_x^e}{\lambda_x^e + \lambda_x^+} \, g \, D_n , \qquad (1)$$

where T_l is the transmission coefficient for l-th partial wave;

${}_nX_x$ is the number of nucleons of type "x" in the n-exciton state; ε_x is the channel energy of the nucleon; $\omega(p,h,E)$ is the density of exciton states with "p" particles and "h" holes ($p+h=n$) at the excitation energy E; U is the final excitation energy, $U=E-Q_x-\varepsilon_x$ and Q_x is the nucleon separation energy; D_n is the "depletion" factor; n_0 is the initial exciton number.

The nucleon emission rate λ_x^e is equal to

$$\lambda_x^e = \frac{(2S_x+1)\,\mu_x\,\varepsilon_x\,\sigma_x^{inv}(\varepsilon_x)}{\pi^2\,\hbar^3\,g_x} \qquad (2)$$

where S_x and μ_x are the spin and reduced mass of the outgoing nucleon of type "x", σ_x^{inv} is the inverse reaction cross-section for particle "x", and g_x is the single-nucleon state density.

The l-depending intranuclear transition rate λ_x^+ is calculated using the nucleon-nucleon scattering cross-section corrected for the Pauli principle and the average nuclear matter density at the distance from $l\lambda\!\!\!^-$ to $(l+1)\lambda\!\!\!^-$. For nucleon induced reactions the density of excited states with the number of excitons with n=2 and 3 is obtained considering the finite depth of the nuclear potential well [5]. The number of nucleons of x-type in the n-exciton state ${}_nX_x$ for is calculated using the ratio of the nucleon-nucleon cross-sections obtained taking into account the Pauli principle and the nucleon motion [4]. Multiple pre-compound nucleon emission is simulated by means of TALYS.

The exciton coalescence model [6,7] and the knock-out model [8] are used for the calculation of pre-equilibrium energy distributions of light clusters, d, t, ^{3}He, and α-particles [4,9]. The contribution of direct processes is taken into account for deuterons using the phenomenological approach [10].

The pre-equilibrium spin distribution is calculated as described in details in Ref.[3].

3. CHANGES IN TALYS AND ALICE/ASH

Six subroutines of TALYS and thirty subroutines of ALICE/ASH were modified and seven new subroutines were written for appropriate integration of GDH algorithm in TALYS.

The value of the TALYS input variable "preeqmode" equal to 5 is responsible now for GDH calculations. Various options of GDH and the hybrid model can be chosen by the user in the subroutine "gdhinput".

4. EXAMPLES OF ENERGY DISTRIBUTIONS OF REACTION PRODUCTS CALCULATED USING GDH MODEL IMPLEMENTED IN TALYS

Several examples of energy distributions of emitted neutrons, protons, deuterons, and α-particles calculated with the help of the GDH and other models implemented in TALYS in the present work are shown in Figs.1-8. For the comparison results of calculations using the default options of the TALYS input block are also shown. Default options suppose the use of the pre-equilibrium exciton model [12] and the approach from Ref.[13] for the modelling of non-equilibrium cluster emission.

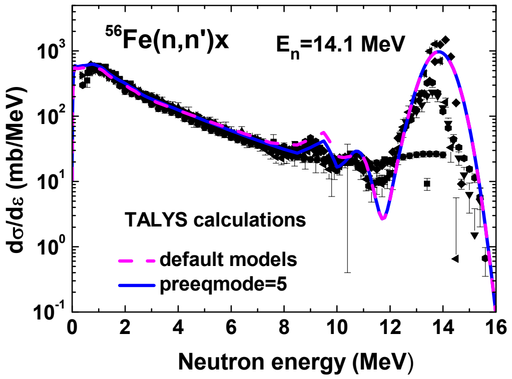

Fig. 1. The energy distribution of neutrons in the ^{56}Fe(n,n')x reaction induced by 14.1 MeV neutrons. Experimental data are taken from EXFOR. "preeqmode=5" refers to calculations using nuclear models implemented in TALYS in the present work.

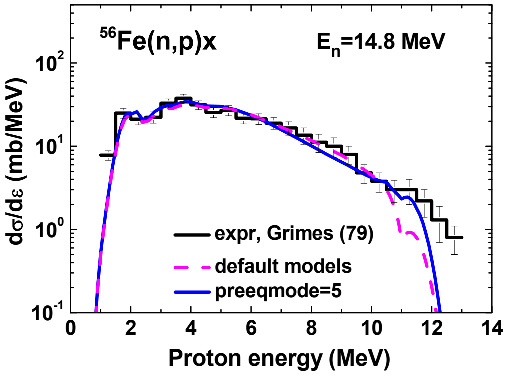

Fig. 2 The energy distribution of protons in the ^{56}Fe(n,p)x reaction induced by 14.8 MeV neutrons. See comments to Fig.1

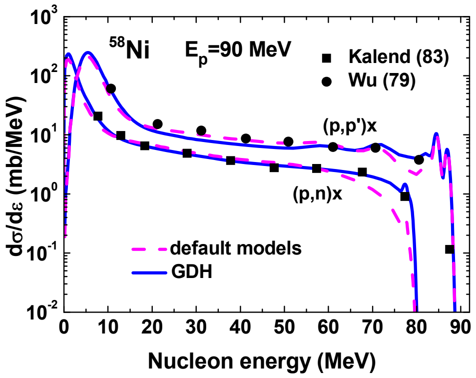

Fig. 3 The energy distribution of nucleons in the p+^{58}Ni reaction induced by 90 MeV protons. See comments to Fig.1

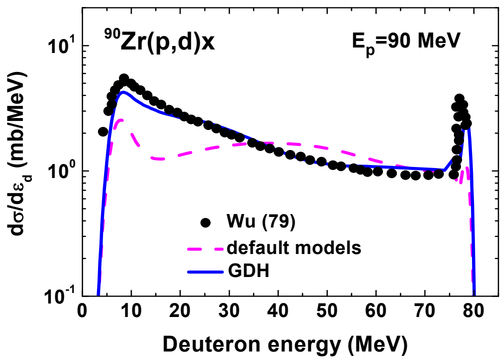

Fig. 6. The energy distribution of deuterons in the ^{90}Zr(p,d)x reaction induced by 90 MeV protons. See comments to Fig.1.

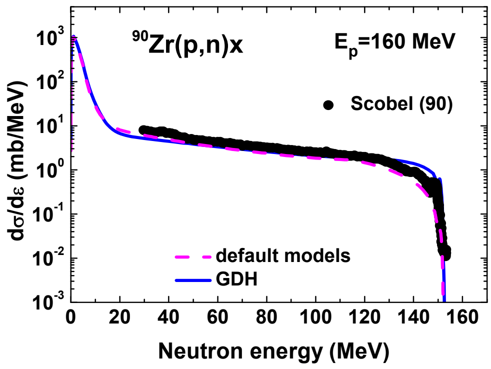

Fig. 4. The energy distribution of neutrons in the ^{90}Zr(p,n)x reaction induced by 160 MeV protons. See comments to Fig.1

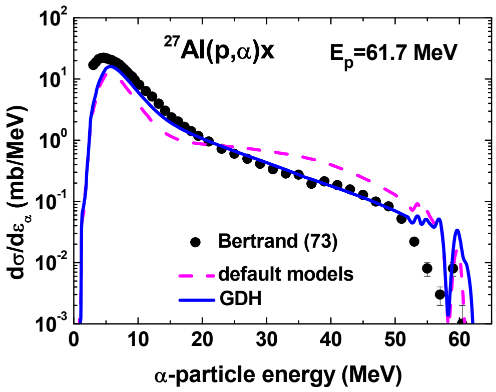

Fig. 7. The energy distribution of α-particles in the ^{27}Al(p,α)x reaction induced by 61.7 MeV protons. See comments to Fig.1

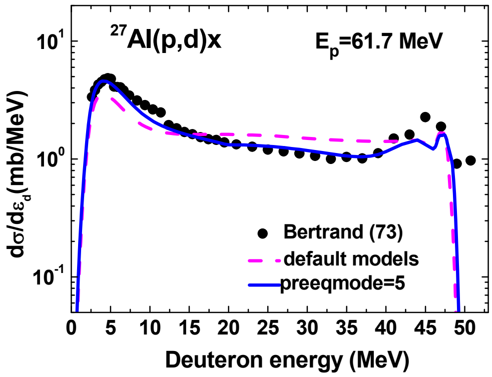

Fig. 5. The energy distribution of deuterons in the ^{27}Al(p,d)x reaction induced by 61.7 MeV protons. See comments to Fig.1

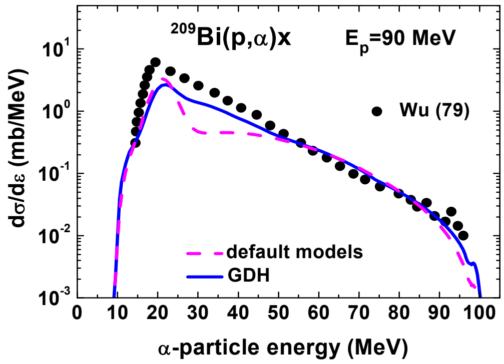

Fig. 8. The energy distribution of α-particles in the ^{209}Bi(p,α)x reaction induced by 90 MeV protons. See comments to Fig.1

5. COMPARISON WITH EXPERIMENTAL (P,X) REACTION CROSS-SECTIONS

The comparison with measured (p,x) reaction cross-sections was performed using several thousands of (Z,A,E_p) experimental points. The ranges of atomic numbers Z of target nuclei is from 12 to 83, mass numbers A from 24 to 209 and the incident proton energies E_p up to 150 MeV. The procedure of the selection and the origin of experimental (p,x) data is discussed in details in Ref.[14].

A number of deviation factors are used for the quantification of the difference between results of calculations and experimental data [14]:

$$H = \left(N^{-1} \sum_{i=1}^{N} \left(w_i^{\exp} - w_i^{calc} \right)^2 \right)^{1/2}, \tag{3}$$

$$R^{CE} = N^{-1} \sum_{i=1}^{N} \frac{\sigma_i^{calc}}{\sigma_i^{\exp}} \tag{4}$$

$$R^{EC} = N^{-1} \sum_{i=1}^{N} \frac{\sigma_i^{\exp}}{\sigma_i^{calc}} \tag{5}$$

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

$$S = 10^{\left\{ \left(\sum_{i=1}^{N} \left[w_i^{\exp} \lg(\sigma_i^{\exp} / \sigma_i^{calc}) \right]^2 \right) \Big/ \left(\sum_{i=1}^{N} \left[w_i^{\exp} \right]^2 \right) \right\}^{1/2}} \tag{7}$$

where $w_i^{\exp} = \sigma_i^{\exp} / \Delta\sigma_i^{\exp}$, $w_i^{calc} = \sigma_i^{calc} / \Delta\sigma_i^{\exp}$, $\sigma_i^{\exp}$ and $\Delta\sigma_i^{\exp}$ are the measured cross-section and its uncertainty, σ_i^{calc} is the calculated cross-section, and N is the total number of experimental points selected for each type of the comparison with the non-zero values of σ_i^{calc}.

The discussion of various deviation factors can be found in Ref.[14].

Table 1 presents the values of H, R^{CE}, R^{EC}, L, and S obtained using results of various sets of calculations. The calculations were performed with the help of the following models: i) the nuclear models including the pre-equilibrium exciton model [3,12] and corresponding to default input options of TALYS, ii) the GDH model implemented in TALYS, iii) GDH model combined with Weisskopf-Ewing model integrated in the ALICE/ASH code.

One can see the noticeable improvement of the quality of predictions for the GDH model combined with Hauser-Feshbach model in comparison with GDH-Weisskopf-Ewing (Table 1, the meaning of factors can be found in Ref.[14]).

Table 1 Values of various deviation factors, obtained using (p,x) reaction cross-sections calculated using various nuclear models and computer programs for target nuclei with the atomic number from 12 to 83 at the incident proton energy up to 150 MeV. The N number is equal to 16045

Factor	TALYS, (default)	TALYS, GDH	ALICE/ASH
H	20.3	20.9	26.8
R^{CE}	1.24	1.27	1.27
R^{EC}	2.33	1.98	831.
L	0.45	0.51	0.60
S	1.34	1.33	2.44

6. CONCLUSION

The geometry dependent hybrid model supplemented by phenomenological models for the modelling of non-equilibrium emission of light clusters was implemented in the TALYS code. Models considered presents the alternative to the pre-equilibrium exciton model integrated in TALYS and can be used for the prediction of cross-sections and distribution of secondary particles in nuclear reactions induced by intermediate energy particles.

The comparison of the GDH model implemented in TALYS and in ALICE/ASH codes shows definite advantage the GDH-Hauser-Feshbach combination.

REFERENCES

[1] M. Blann, *Phys. Rev. Lett.*, **28**, 757(1972).

[2] M. Avrigeanu, V. Avrigeanu, "STAPRE-H95," NEA Data Bank, IAEA0971, 1996.

[3] A. J. Koning, S. Hilairey, and M. Duijvestijn, "TALYS-1.0" (2007); http://www.talys.eu/

[4] C. H. M. Broeders, A. Yu. Konobeyev, Yu. A. Korovin, V.P. Lunev, M. Blann, "ALICE/ASH," FZKA 7183, Forschungszenrum Karlsruhe (2006), http://bibliothek.fzk.de/zb/berichte/FZKA7183.pdf

[5] M. Blann, *Phys. Rev.*, **C54**, 1341(1996).

[6] A. Iwamoto, K. Harada, *Phys. Rev.*, **C26,** 1821(1982).

[7] K. Sato, A. Iwamoto, K. Harada, *Phys. Rev.,* **C28**, 1527 (1983).

[8] A. Yu. Konobeyev, V. P. Lunev, Yu. N. Shubin, *Acta Physica Slovaca,* **45**, 705(1995).

[9] A. Yu. Konobeyev, A. Yu. Korovin, *Kerntechnik,* **59**, 72 (1994).

[10] C. H. M.Broeders, A. Yu. Konobeyev, *Kerntechnik,* **70**, 260 (2005).

[11] P. Obložinský, I. Ribanský, *Phys. Lett.,* **74B**, 6(1978).

[12] A. J. Koning, M. C. Duijvestijn, *Nucl. Phys.,* **A744**, 15(2004).

[13] C. Kalbach, *Phys. Rev.,* **C71**, 034606(2005).

[14] A. Yu. Konobeyev, U. Fischer, A. J. Koning, H. Leeb, S. Leray, Y. Yariv, "What Can We Expect from the Use of Nuclear Models Implemented in MCNPX at Projectile Energies below 150 MeV? Detailed Comparison with Experimental Data", this Conference.