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Letter to the Editor

Improvement in simulation of equilibrium particle emission using intranuclear cascade evaporation model

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Abstract

The modified intranuclear cascade evaporation model combining the Monte Carlo method for the simulation of non-equilibrium particle emission and deterministic algorithm for the description of equilibrium de-excitation is discussed. The nuclear level density for equilibrium states is calculated using the generalized superfluid model taking into account shell and collective effects. The inverse reaction cross-sections are calculated by the nuclear optical model. The model was used for the analysis of radionuclide yields in proton-induced reactions at energies 0.8–2.6 GeV. The results of calculations show the advantage of the model proposed in accuracy of predictions compared with other popular intranuclear cascade evaporation models.

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1. Introduction

During last decades intranuclear cascade evaporation model was successfully used for the prediction of nuclear reactions characteristics: energy and angular distributions of emitted particles, excitation functions, yields of fission fragments, residual recoil spectra and others.

The model consists of two parts, whose development historically occurred independently of each other: the intranuclear cascade model, which describes non-equilibrium processes in the nucleus, and statistical evaporation model. Progress in the description of intranuclear interactions is connected, mostly, to create the "time-dependent" models [1,2], the approaches modelling in detail the density distribution of nucleons in the nucleus [2,3], the combination of the intranuclear cascade and precompound exciton models [4] and with the development of the model considering the interactions with "preformed" clusters [5].

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Traditionally, a number of approximations was used in the simulation of equilibrium process, whose need was caused by limited power of computers. The use of the simplest models for calculating the nuclear level density [6,7], the "sharp-cut-off" approach to the inverse reaction cross-section calculation [7–9], other simplifications, which make it possible to obtain analytical expressions for calculating particle emission widths [10,11], can be attributed to these approximations. The simplified models are used in all popular codes implementing the intranuclear cascade evaporation model [11,12]. At the same time, modern computer technology makes it possible to use more rigorous and advanced models for the simulation of the equilibrium particle emission using intranuclear cascade evaporation model.

This paper describes the intranuclear cascade evaporation model avoiding the lack of usual simplifications [6–12] in the modelling of equilibrium particle emission. The nuclear level density is calculated using the generalized superfluid model with parameters fitted to cumulative number of low-lying levels and observed neutron resonance densities [13,14]. Inverse reaction cross-sections are obtained by the optical model without "sharp-cut-off" approximation. No simplification is made to get particle emission widths at low and high energy of excitation.

The proposed intranuclear cascade evaporation model is used for the calculation of the radionuclide yields in nuclear reactions induced by protons with energy of 0.8–2.6 GeV. The results are compared with experimental data and calculations performed using different intranuclear cascade evaporation models [12]: the Dresner [15] and ABLA [16] evaporation models combined with the Bertini [17], ISABEL [1,18] and INCL4 [3] intranuclear cascade models, as with help of the CEM2k [12,19] and CASCADE [2,20] models.

2. Model description

2.1. Equilibrium model

The modelling of equilibrium emission is performed without the consideration of angular momentum, which is the simple consequence of the limited power of computers. The particle emission rate is calculated as follows [21]:

$$W_x(\varepsilon_x) = \frac{(2S_x+1)\mu_x\varepsilon_x}{\pi^2\hbar^3}\,\sigma_x^{\mathrm{inv}}(\varepsilon_x)\,\frac{\rho(Z',A',U)}{\rho(Z,A,E)} \tag{1}$$

where S_x, μ_x and ε_x are, respectively, spin, reduced mass and energy of the emitted particle, σ_x^{inv} the inverse reaction cross-section, $\rho(Z',A',U)$ the nuclear level density for residual nucleus with the excitation energy U, $\rho(Z,A,E)$ the level density for the nucleus emitting the x-particle, and E the excitation energy.

The nuclear level density is calculated according to the generalized superfluid model [13]

$$\rho(U) = \rho_{\mathrm{qp}}(U')K_{\mathrm{vib}}(U')K_{\mathrm{rot}}(U') \tag{2}$$

where $\rho_{\mathrm{qp}}(U')$ is the density of quasi-particle nuclear excitation [13], and $K_{\mathrm{vib}}(U')$ and $K_{\mathrm{rot}}(U')$ are the vibrational and rotational enhancement factors at the effective energy of excitation U' calculated, respectively, according to Refs. [14,22].

The nuclear level density parameters are calculated according to the following expression [13]:

$$a(U) = \begin{cases} \tilde{a}(1+\delta W\,\varphi(U'-E_{\mathrm{cond}})/(U'-E_{\mathrm{cond}}), & U'>U_{\mathrm{cr}} \\ a(U_{\mathrm{cr}}), & U'\leqslant U_{\mathrm{cr}} \end{cases} \tag{3}$$

where δW is the shell correction to the mass formula equal to the difference between experimental mass defect and one calculated from the liquid drop model [23], $\varphi(U) = 1-\exp(-\gamma U)$, $\gamma = 0.4/A^{1/3}\,\mathrm{MeV}^{-1}$. The asymptotic value of nuclear level parameter is given as

$$\tilde{a} = A(0.073 + 0.115A^{-1/3}). \tag{4}$$

The effective energy of excitation U', the critical energy of the phase transition U_{cr} and the condensation energy E_{cond} are calculated as follows:

$$U' = U - n\Delta_0 \tag{5}$$

$$U_{\mathrm{cr}} = 0.472\,a(U_{\mathrm{cr}})\Delta_0^2 - n\Delta_0 \tag{6}$$

$$E_{\mathrm{cond}} = 0.152\,a(U_{\mathrm{cr}})\Delta_0^2 - n\Delta_0. \tag{7}$$

The correlation function Δ_0 is equal to

$$\Delta_0 = 12A^{-1/2} \tag{8}$$

where $n = 0$ for even–even nuclei, $n = 1$ for nuclei with odd A value, $n = 2$ for odd–odd nuclei.

The inverse reaction cross-section σ_x^{inv} is calculated by the optical model. The parameters of the optical potentials for nucleons and light charged fragments are discussed in Refs. [24,25]. The calculated σ_x^{inv} cross-section values are used in the integration of particle emission rates, Eq. (1).

The probability of the photon emission is calculated according to Weisskopf–Ewing model [21] with the photon absorption cross-section parameterized in Ref. [26]. The fission probability is calculated using the Bohr–Wheeler approach [27]. The distribution of fission fragments is calculated according to Ref. [28].

The discussed model is implemented in the computer code following Refs. [29,30]. The non-equilibrium particle emission is modelled by the Monte Carlo method using the intranuclear cascade model. The emission of fast particles for each Monte Carlo history results in the creation of residual nucleus with a certain atomic and mass numbers Z, A, with the excitation energy U. For the residual nucleus (Z, A, U) the calculation of reaction products is performed using the "deterministic" algorithm by the common integration of particle emission rates, without resorting to Monte Carlo. This method is more time consuming than usual intranuclear cascade evaporation algorithm, but that less consuming than the deterministic integration of all non-equilibrium and equilibrium particle emission rates. The advantage of the method is its relative simplicity and fast implementation in the computer code, since the routines describing the equilibrium emission in the widely used and verified computer codes, as STAPRE [31], GNASH [32], ALICE [33], etc. can be used for this purpose.

In the present work the calculations are performed using the equilibrium algorithm from the modified ALICE code [33].

2.2. Non-equilibrium model

The non-equilibrium particle emission is described using the intranuclear cascade model implemented in the CASCADE (Dubna) code [20]. Below, this model combined with the equilibrium model described in Section 2.1 is denoted by CASCADE/ASF.

3. Comparison of calculations with experimental data

The detail and adequate information, which can be used for the demonstration of predictive power of the equilibrium model combined with intranuclear cascade model, are the measured yields of radionuclides. By the principle of "random selection" we take the results of recent measurements of the radionuclide yield in the irradiation of ^{59}Co and ^{184}W by protons with the energy from 0.8 to 2.6 GeV [34].

The calculations were performed using the model discussed in Section 2 and by various intranuclear cascade evaporation models: the CASCADE [2,20] and CEM2k [12,19] models, the Bertini [17], ISABEL [18] and INCL4 [3] models combined with the Dresner [15] and ABLA [16] evaporation models. All four evaporation models considered (Dresner, ABLA, CASCADE and CEM2k) use certain approximations in the modelling of equilibrium particle emission: the Fermi gas model for the level density calculation [6,7,10,12], the "sharp-cut-off" formulas for inverse cross-sections [8], and other simplifications justified only at high-excitation energies [10].

The calculated radionuclide yields were normalized on the values of the non-elastic cross-sections for proton interactions with nuclei, calculated by MCNPX [12] (Tables 1 and 2). An equal number of Monte Carlo histories was used in the simulations by different models. The cumulative cross-sections were obtained using the decay data from FENDL/D-2. The unknown isomeric cross-section ratios were taken to be 0.5.

The quantification of the agreement between calculations and measured data has been done using the F-deviation factor [6,34,36]

$$F = 10^{\left(\frac{1}{N}\sum_{i=1}^{N}[\log(\sigma_i^{\text{exp}})-\log(\sigma_i^{\text{calc}})]^2\right)^{1/2}}. \tag{9}$$

Table 1
Results of the comparison of experimental data [34] with calculations for ^{59}Co irradiated with 1.2–2.6 GeV protons

Factor	Bertini/ Dresner	Bertini/ ABLA	ISABEL/ Dresner	ISABEL/ ABLA	INCL4/ Dresner	INCL4/ ABLA	CEM2k	CASCADE (original)	CASCADE/ ASF (this work)
Proton energy 1.2 GeV, number of points 20, $\sigma_{non} = 772$ mb									
H	4.87	15.85	4.58	21.17	4.16	20.35	6.52	12.79	6.02
D	0.32	0.81	0.28	1.10	0.25	1.02	0.41	0.60	0.36
R	0.70	1.50	0.89	1.83	0.91	1.78	0.93	1.12	1.10
F	1.74	2.07	1.58	2.31	1.56	2.21	1.78	2.52	*1.50*
Proton energy 1.6 GeV, number of points 20, $\sigma_{non} = 773$ mb									
H	4.51	13.79	5.66	23.16	4.30	20.05	5.82	11.80	5.51
D	0.33	0.81	0.33	1.27	0.25	1.13	0.37	0.59	0.37
R	0.71	1.43	1.01	2.04	0.95	1.87	0.84	1.11	1.09
F	1.96	2.11	1.65	2.45	1.51	2.30	1.78	2.38	*1.48*
Proton energy 2.6 GeV, number of points 20, $\sigma_{non} = 770$ mb									
H	4.29	13.71	5.78	28.15	4.42	26.00	5.23	10.26	5.51
D	0.32	0.80	0.34	1.63	0.27	1.45	0.36	0.58	0.37
R	0.71	1.42	1.15	2.38	1.03	2.23	0.80	1.08	1.08
F	1.76	2.11	1.55	2.75	*1.47*	2.55	1.86	2.31	1.49
All energies, number of points 60									
H	4.56	14.48	5.37	24.34	4.29	22.30	5.88	11.66	5.69
D	0.32	0.81	0.32	1.33	0.26	1.20	0.38	0.59	0.37
R	0.71	1.45	1.02	2.08	0.96	1.96	0.86	1.10	1.09
F	1.82	2.10	1.59	2.50	1.51	2.35	1.81	2.40	*1.49*

The cross-section of non-elastic proton interaction σ_{non} is shown. The best results are in italics.

Table 2
Results of the comparison of experimental data [34] with calculations for ^{184}W irradiated with 0.8 and 1.6 GeV protons

Factor	Bertini/ Dresner	Bertini/ ABLA	ISABEL/ Dresner	ISABEL/ ABLA	INCL4/ Dresner	INCL4/ ABLA	CEM2k	CASCADE (original)	CASCADE/ ASF (this work)
Proton energy 0.8 GeV, number of points 67, $\sigma_{non} = 1636$ mb									
H	5.08	5.04	5.05	5.35	5.56	6.18	4.85	4.72	4.34
D	0.38	0.39	0.37	0.38	0.41	0.43	0.38	0.39	0.33
R	0.83	0.83	0.78	0.78	0.75	0.75	0.80	0.78	0.86
F	1.76	2.28	2.13	2.24	2.20	2.54	2.89	1.65[a]	*1.57*
Proton energy 1.6 GeV, number of points 91, $\sigma_{non} = 1687$ mb									
H	6.89	5.67	5.45	5.91	5.25	6.08	5.88	4.90	4.51
D	0.48	0.44	0.44	0.44	0.38	0.40	0.45	0.35	0.33
R	0.87	0.89	0.80	0.83	0.79	0.85	0.89	0.83	0.87
F	1.87	2.63	2.60	2.83	2.73	2.57	3.60	2.85[b]	*1.69*
All energies, number of points 158									
H	6.19	5.41	5.28	5.68	5.38	6.12	5.47	4.82	4.44
D	0.44	0.42	0.41	0.41	0.39	0.41	0.42	0.37	0.33
R	0.85	0.86	0.79	0.81	0.77	0.81	0.85	0.81	0.87
F	1.82	2.48	2.40	2.58	2.51	2.56	3.30	2.39[c]	*1.64*

The cross-section of non-elastic proton interaction σ_{non} is shown. The best results are in italics.

[a]Number of points (N) is equal to 58.
[b]N is equal to 86.
[c]N is equal to 144.

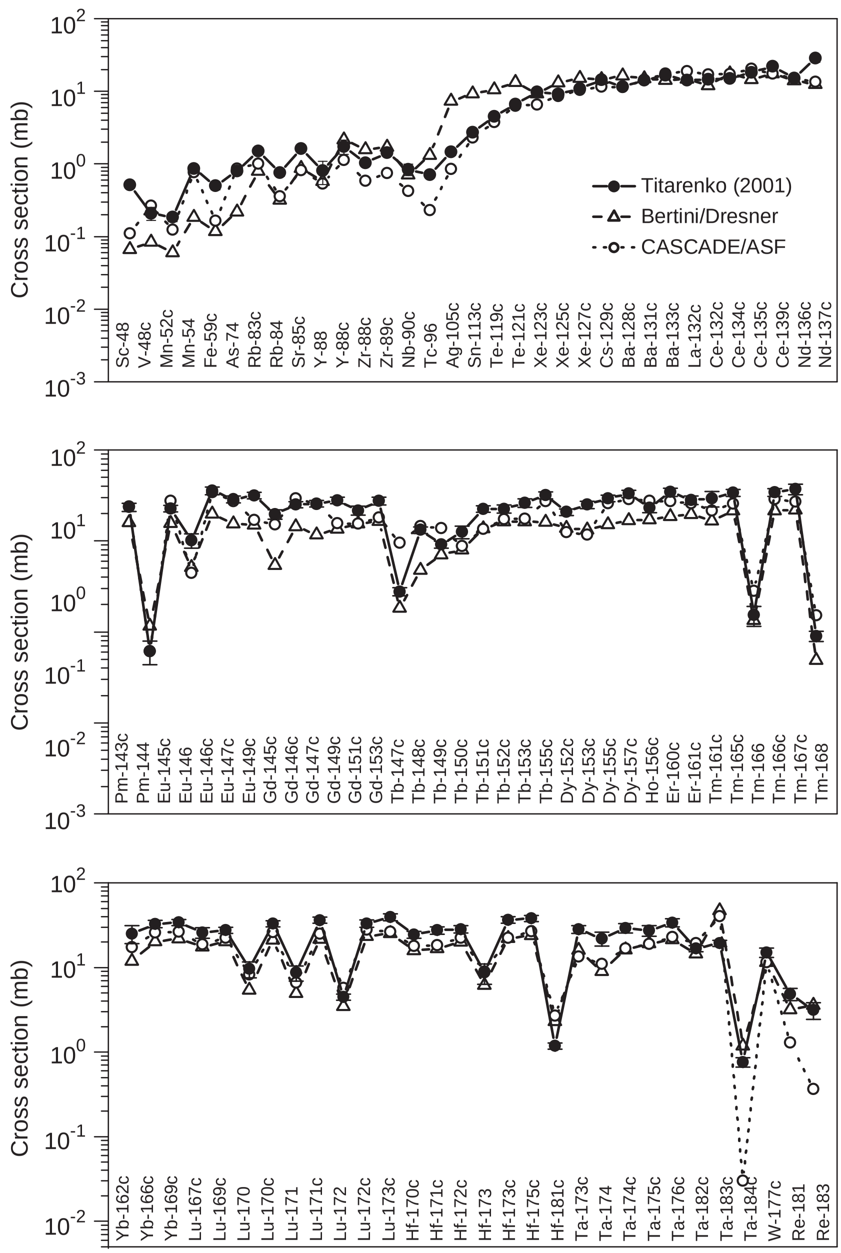

Fig. 1. The radionuclide production cross-sections calculated by the proposed CASCADE/ASF model and the Bertini/Dresner model for ^{184}W irradiated with 1.6 GeV protons and measured in Ref. [34]. Cumulative yields are indicated. If the calculated value is absent, it coincides with the experimental point. The difference between two calculations for residual nuclei with atomic mass number close to 184 is rather due to the difference in intranuclear cascade models and not in evaporation ones.

For illustration purposes one can use also other deviation factors [35]

$$H = \left(\frac{1}{N} \sum_{i=1}^{N} \left(\frac{\sigma_i^{\exp} - \sigma_i^{\text{calc}}}{\Delta\sigma_i^{\exp}} \right)^2 \right)^{1/2} \tag{10}$$

$$D = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{\sigma_i^{\exp} - \sigma_i^{\text{calc}}}{\sigma_i^{\exp}} \right| \tag{11}$$

$$R = \frac{1}{N} \sum_{i=1}^{N} \frac{\sigma_i^{\text{calc}}}{\sigma_i^{\exp}} \tag{12}$$

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

The F-criterion [6,34,36], Eq. (9) is the most adequate for the comparative analyses of different calculations, taking into account that the measured yields are known only for the limited number of residual nuclei. In this case, the F-factor reproduces the systematic underestimation as the overestimation of the results of calculations compared with experimental data. In other criteria, Eqs. (10)–(12) the underestimation of the σ_i^{calc} values has an "advantage" compared with overestimation of the results. For this reason, in spite of the clarity of Eq. (10)–(12), these criteria are of secondary importance and used in the present paper for an illustrative purpose only.

Tables 1 and 2 show the values of different deviation factors obtained from the comparison of calculations with the experimental data [34]. Taking into account, that the use of the systematics Eq. (4) is justified for medium and heavy nuclei, the consideration is limited by the yields of residual nuclei with $Z>20$. For an illustration, Fig. 1 shows the absolute values of radionuclide yields calculated by the proposed CASCADE/ASF model and the Bertini/Dresner model and measured in Ref. [34] for ^{184}W irradiated with 1.6 GeV protons.

The comparison shows that the substitution of the original evaporation algorithm in the CASCADE code [2,20] by the model described in Section 2 results in a noticeable gain in accuracy of predictions. In most cases the model discussed is also the best compared with other models (Tables 1 and 2, Fig. 1).

4. Conclusion

The modified intranuclear cascade evaporation model combining the Monte Carlo method for the simulation of non-equilibrium particle emission and deterministic algorithm for the description of equilibrium de-excitation was discussed. The nuclear level density for equilibrium states was calculated using the generalized superfluid model taking into account collective enhancement of the nuclear level density in addition to shell and superfluid effects [13,14]. The inverse reaction cross-sections were calculated by the nuclear optical model. Calculations were performed without additional simplifications [10,11], usually applied in the simulation of evaporation particle cascade at high energies.

The proposed model has been used for the analysis of radionuclide yields in the proton-induced reaction at energies 0.8–2.6 GeV. The results of calculations show the definite advantage of the model in accuracy of predictions in comparison with other intranuclear cascade evaporation models [12,20].

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