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Development of the Monte Carlo model CASCADE-2004 of high-energy nuclear interactions

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Abstract. The Monte Carlo code CASCADE for the calculation of inelastic hadron- and nucleus-nucleus interactions at energies from several tens of MeV up to several tens of GeV and for modelling of nuclear-physical processes accompanying the transport of particles and nuclei in matter is improved by considering a more detailed model of decay of highly excited residual (after-intranuclear-cascade) nuclei. Results of calculations are in good agreement with experiment. However, there are some deviations for light-isotope production, which prompt the necessity of developing more correct models of evaporation and strong asymmetric high-energy fission.

PACS. 24.10.Lx Monte Carlo simulations (including hadron and parton cascades and string breaking models) – 24.60.Dr Statistical compound-nucleus reactions – 24.75.+i General properties of fission – 24.10.Pa Thermal and statistical models

1 Introduction

Many important applied problems —for example, the study of accelerator-driven nuclear reactors for the production of energy and transmutation of radioactive waste, the design of shielding for accelerators and space vehicles, the use of particle beams for cancer therapy, etc.— demand mathematical modeling of high-energy particle transport in media and accompanying physical effects. Experiments in these regions are rather complicated and expensive, so in many cases such calculations are only one way to get information, as the considered systems have a complicated geometrical structure with heterogeneous density. The Monte Carlo method is the most convenient one for the calculations allowing one to take into account practically all details of the experiments.

Several Monte Carlo codes are developed for such investigations, particularly LAHET (cascade - pre-equilibrium - evaporation fission code) [1] and its generalization LAHET/GEM [2–4], CASCADE (cascade - pre-equilibrium - evaporation fission code) [5–7] developed in Dubna with its modifications SONET [8], SHIELD [9], CEM2k (Cascade-Exciton Model code) + GEM2 [10], INCL4 (Intra-Nuclear-Cascade-Liège) [11].

The LAHET code provides two options for handling intranuclear cascades. As an alternative to Bertini's model (default), it has the ISABEL version of the Intra-Nuclear Cascade (INC), which allows one to treat also nucleus-nucleus interactions. In the ISABEL INC models, the nuclear density is approximated by up to 16 discrete bins, rather than by three bins as in the Bertini INC code and seven bins in the Dubna version of the CASCADE code. In CASCADE, hadron interactions are sampled by means of tables of phenomenological parameters [5,7] taking into account the energy-momentum conservation law and decreasing of intranuclear density due to a knock-out of nucleons [12]. The latter effect is especially important at high energies and in nucleus-nucleus collisions where many intranuclear interactions happened.

In the Dubna INC code the matter density is described by a Fermi distribution with the parameters taken from the electron-nucleus scattering experiment. For simplicity, the nuclear density is considered constant in the seven bins. The CASCADE code takes into account the energy-momentum conservation statistically, not at each step of the cascade. It uses the Pauli exclusion principle which forbids a number of intranuclear collisions and effectively increases the mean free path of cascade particles inside the target. The interaction of the incident particle with the nucleus is approximated as a series of successive quasifree collisions of the fast-cascade particles (N or π) with intranuclear nucleons. To describe these collisions the code uses an elementary cross-section of NN and πN of the free particles, simulating angular and momentum distributions of

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secondary particles using special polynomial expressions with energy-dependent coefficients taking into account the Pauli principle [7]:

$$NN \to NN, NN \to \pi NN, NN \to \pi_i NN, \pi N \to \pi N, \pi N \to \pi_i N, \qquad (i \geq 2)\,. \tag{1}$$

Cross-sections of the hadron-nucleus collisions in our code are calculated based on the compilations of the experimental data [13,14]. To calculate the nucleus-nucleus cross-sections, we use analytical approximations with parameters defined in comparison with experiment [13,15]. Except for the elementary processes, the Dubna INC also takes into account pion absorption on nucleon pairs,

$$\pi NN \to NN\,. \tag{2}$$

The momenta of two nucleons participating in the absorption are chosen randomly from the Fermi distribution, and the pion energy is distributed equally between these nucleons in the center-of-mass system of the pion and nucleons participating in the absorption. The direction of the motion of the resultant nucleons in this system is taken as isotropically distributed in space. The effective cross-section for absorption is similar (but not equal) to the experimental cross-sections for pion absorption by deuterons. Due to large ionization losses, low-energy charged particles in intranuclear showers can be considered, in most cases, as stopped. The respective cutoff energies are 2 MeV for π^+-mesons (low-energy π^--mesons are captured by nuclei generating intranuclear cascades), 10 MeV for protons and deuterons, 30 MeV for tritons and 10 MeV/nucleon for all heavier ions. However, for biophysical problems, the investigation of the radiation damage to microelectronic devices and some other applications, where a large radiation damage produced by low-energy particles is important, one must consider lower cutoff energies [16]. Possible decays of π-mesons are also taken into account. A detailed comparison of the Dubna INC with the well-known Bertini INC developed at Oak Ridge National Laboratory [17] and with the popular version developed at Brookhaven National Laboratory and Columbia University by Chen *et al.* [18] is made in ref. [19].

In CASCADE, the decay of a after-cascade nucleus includes three processes: a relaxation of the high-excited nucleus, accompanied by a possible emission of nucleons and light fragments (pre-equilibrium decay), to an equilibrium state; the decay of this state due to the competition of particle evaporation and fission; and, finally, hadron and light-fragment evaporation from fragments of the fission nucleus may occur if they have enough excitation energy. Monte Carlo modelling of the evaporation and fission is described in the next two sections. It is supposed that the residual several MeV of the excitation are taken by emitted γ quanta.

In LAHET, the transition from the fast-cascade stage to the pre-equilibrium stage is defined by the cutoff energy. The value of the neutron cutoff energy is randomly chosen between zero and twice the mean binding energy. For protons, this code assumes a cutoff energy that is equal to the larger of the two, the Coulomb barrier or the neutron cutoff energy. In CASCADE this energy is defined by the binding energy of the nucleon plus some energy defined phenomenologically (see details in refs. [5,6]).

The pre-equilibrium stage in LAHET is modeled by the multistage multistep exciton model (MPM) and allows one to handle the formation of composite particles like neutrons protons, deuterons, tritons, ^{3}He and ^{4}He particles before statistical equilibrium is reached. The relaxation in the pre-equilibrium stage is considered on the basis of the Blann model [20,21].

De-excitation of the excited nuclei by fission/evaporation in the LAHET code is described optionally by i) RAL's fission model by Atchinson [22], ii) ORNL version [23] and the Dresner evaporation code [24] based on the Weisskopf-Ewing approach.The disintegration of light nuclei ($A < 20$) can be modeled optionally by the Fermi breakup model. In case of RAL's model, good or bad agreement of the calculations with experiment interprets nothing on the mechanism of nuclear fission and characterizes only the quantity of the used approximations. Such an approach is worth considering for applied problems, connected with particle transport in matter; however, it is unsufficient for physical investigations. The CASCADE code uses a macroscopic description of fission based on the liquid-drop model [7,25,26]. By use of fission models the agreement with experimental charge-mass distributions of produced isotopes, as a rule, is somewhat worse, especially for high- and low-mass nuclei (strong asymmetric fission). In INCL4, the evaporation and fission processes are described by the ABLA code [27].

To describe low-energy neutron interactions, all these codes use the multigroup constants tested in reactor physics. The neutrons with energies less than 10.5 MeV are considered by means of 26-group constants [28]. The use of more detailed constant sets is important for modelling of transmutation processes and isotope distribution in low-energy fission.

The goal of our paper is to describe the improvements of the model for the decay of excited residual nuclei (particularly for their fission), which allow one to get better agreement of the CASCADE code calculations with experiment and can be applied to other codes being used now.

2 Description of the evaporation model

Instead of the simple approximation for the Fermi-gas level density

$$\rho(U) = C \exp\left(\sqrt[2]{a(U-\Delta)}\right) \tag{3}$$

with constant value of parameter a used in the previous versions of CASCADE, we use now a more precise expression,

$$\rho(U) = C_1 (U-\Delta)^{-5/4} a^{-1/4} \exp\left(\sqrt[2]{a(U-\Delta)}\right), \tag{4}$$

for the excitation energies $U > E_b$ and

$$\rho(U) = C_2 \exp{(U - E_1)/T}\,, \tag{5}$$

if $U < E_b$. The boundary energy $E_b = E_0 + \Delta$, where $E_0 = 2.5 + 150/A_d$ and A_d is the decayed (daughter) nucleus mass number. The parameter $1/T$ is of the form $\sqrt{a/E_0} - 1.5/E_0$ [29,30] and $E_1 = E_b - T(\log T - 0.25\log a - 1.25\log E_0 + 2\sqrt{aE_0})$. The constant C_2 is defined by the condition of the equality of the densities (4) and (5) at the point $U = E_b$. The pairing energy shift Δ is defined according to the tables [29,30]. For the level density parameter we use the expression [31–33]

$$a(A_d, Z_d, U) = A_d(0.134 - 1.21 \cdot 10^{-4} A_d)(1 + (S/U) \times (1 - \exp(-0.061U))). \quad (6)$$

Here A_d and Z_d are the mass and charge numbers of the decayed nucleus, U is the decaying (parent) nucleus excitation energy (MeV), S is the shell correction [29].

The evaporation probability for the particle (or fragment) i is defined by the expression (in units of $\hbar = c = 1$)[1]

$$P_i = (2/\pi) m_i (2s_i + 1) \int_{V_i}^{U_i - B_i} \sigma_i(E) \rho(U_i - B_i - E) E \mathrm{d}E, \quad (7)$$

where s_i and m_i are the spin and mass of the evaporated particle. For the binding energy B_i we use the values from the tables in ref. [34]). U_i is the excitation energy of the decaying nucleus. The cross-section of the inverse reaction is defined as

$$\sigma(E) = \pi R^2 \alpha (1 + \beta/E) \quad (8)$$

with the constants α and β taken from [4] and $R = 1.5(A_i^{1/3} + A_d^{1/3})$, where A_i is the evaporating-particle mass number. The Coulomb barrier is of the form

$$V_i = 1.44 C_i T_i Z_i (Z - Z_i)/((1.2 A_i^{1/3} + 1.7 A_d^{1/3})) \text{ (MeV)}, \quad (9)$$

where C is the constant proposed by S. Furihata [4] and depends on the charge number of the emitted particle Z_i; A and Z are the mass and charge numbers of the decaying nucleus. As before, A_d is the mass number of the decayed (daughter) nucleus. Coefficient

$$T_i = \begin{cases} 1/(1 + \sqrt{(U/20a_d)}), & U > 200 \text{ MeV}, \\ 1, & U \leq 200 \text{ MeV} \end{cases} \quad (10)$$

with the level density parameter a_d takes into account the empirical temperature dependence.

As the level density parameter is energy dependent, the probabilities of evaporation (and fission, see below) are calculated by means of numerical integration instead of the customary use of some approximate expressions. The sampling of the energy of a particle emitted by the residual nucleus must be done taking into account eqs. (4)-(10). Such a sampling is rather complicated; however, the calculated, emitted particle energies are close to those calculated by the use of the simple equation (3). In most cases one may restrict oneself to the evaporation of six particles: n, p, d, t, ^{3}He, ^{4}He. The heavier fragments are important only in considering the isotope production and other particular problems. Calculation of such fragments is time consuming, because one must take into account the emission of fragments in various excited (resonance) states which must be considered as independent states. How to take into account heavy fragments was shown by S. Furihata [2–4]. Otherwise the light-isotope cross-sections will be essentially underestimated.

[1] As the Monte Carlo sampling uses relative probabilities, the normalization factor, which is common for all evaporation channels and for fission, can be omitted.

3 Simulation of fission

The probability of fission is of the form

$$P_f = \int_0^{U_f - B_f} \rho(U_f - B_f - \Delta_f - E)\, \mathrm{d}E, \quad (11)$$

where the fission barrier B_f [35] is defined as the difference of the saddle point and ground-state nucleus mass. The pairing energy correction is taken as

$$\Delta_f = 14\chi/\sqrt{A} \quad (12)$$

with $\chi = 2, 1, 0$ for even-even, even-odd and odd-even, odd-odd nuclei, respectively.

The evaporation probability (7) and fission probability (11) are used for the sampling of the competition between these reaction channels. Calculations have shown that the agreement with experiment becomes better if in the level density parameter $a_f(A, Z, E)$ is taken a little higher than in eq. (6) which is similar to as given in ref. [22]:

$$a_f = a \begin{cases} 1.1486 + 1.00918 \cdot 10^{-2} F^2 \\ \qquad - 6.5931 \cdot 10^{-4} F^3, \quad Z \leq 85, \\ 1.06253 + 0.9337 \cdot 10^{-2} F^2 \\ \qquad - 6.1 \cdot 10^{-4} F^3, \quad Z > 85 \end{cases} \quad (13)$$

with $F = Z^2/A - 30.893$. The above equation (13) is similar to the one used in RAL's parameterized model and adjusted according to our model to reproduce the experimental data. When a_f is greater than a_n [36], then it takes into account the temperature dependence of the fission barrier B_f.

The masses, charges, kinetic and excitation energies of fragments are determined on the basis of Fong statistical theory of fission [7,37]. The calculated fragment excitation energy is $U = \Delta M - D_1 - D_2 - V$. We assume that the deformation energies D_i are described by the liquid-drop model. The Coulomb potential is given as

$$V = 1.107 Z_1 * Z_2 / \sum_{i=1,2} (G_{1i} + G_{2i}), \quad (14)$$

Table 1. Neutron yield in the lead target with radius R and length L irradiated with protons with energy E.

$R = 5.1$ cm,	$L = 61$ cm		$R = 10.2$ cm,	$L = 61$ cm
E, GeV	Exp. [38,39]	Theor.	Exp. [40]	Theor.
0.47	8 ± 0.4	7.1	8.7 ± 0.4	7.4
0.47	6.4 ± 0.3			
0.72	11.8 ± 0.6	12.0	13.9 ± 0.7	14.2
0.72	11.7 ± 0.4			
0.96	16.6 ± 0.8	17.5	20.3 ± 1.1	20.7
1.47	26.4 ± 1.3	27.9	31.5 ± 1.6	30.9
1.47	27.5 ± 0.6			

Table 2. Neutron yield in the uranium target with radius $R = 10.2$ cm and length $L = 61$ cm irradiated with protons with energy E.

E (GeV)	Exp. [40]	Theor.
0.47	18.1 ± 0.9	14
0.72	29.1 ± 1.5	28
0.96	40.5 ± 2	38
1.47	56.8 ± 2.8	60

where

$$G_{1i} = 1 + \alpha_{2i}(1 - 3\eta_i/5) + \alpha_{3i}(1 - 3\eta_i^2/7)A_i^{1/3}, \quad (15)$$

$$\eta_i = 1.3A_i^{1/3} \sum_{i=1,2} 1.3A_i^{1/3}(1 + \alpha_{2i} + \alpha_{3i} - (9/35)\alpha_{2i}\alpha_{3i}). \quad (16)$$

Here, α_{2i} and α_{3i} are the deformation parameters which have been calculated according to refs. [7,37], A_i, $i = 1, 2$, are the masses of the fission fragments. Calculating the difference of the fissioning nucleus and fragment mass defects ΔM, we use their experimental values [34] or, when such values are unknown, the mass defects are defined by means of Cameron mass formula and the correction tables in ref. [29].

In order to calculate the properties of the fission fragments we need the total density of the quantum states at the scission point. In the original Fong theory of fission, the complete equilibrium has been assumed and this density is defined as

$$\Omega(U) = C \int_0^U \exp\left(\sqrt[2]{(a_1 + a_2)(U_1 + U_2)}\right) \mathrm{d}U_1. \quad (17)$$

However, strong evidence has been found for different thresholds of the symmetric- and asymmetric-fission components [41,42], which demonstrate the influence of the saddle point configuration on the fission fragment distribution. The competition of different fission components as a function of the excitation energy has been explained by the temperature dependence of the shell effects [42,43]. It seems that the population of the fission valleys is determined before reaching the scission configuration or that the complete equilibrium does not occur while deciding the fission fragment distribution. This prompts that one must exclude the complete-equilibrium condition from the Fong theory and take into account separately all partial fragment level densities:

$$\Omega(U) = C \int_0^U \exp\left(\sqrt[2]{a_1(U_1 - \Delta_1)}\right) \times \exp\left(\sqrt[2]{a_2(U - U_1 - \Delta_2)}\right) \mathrm{d}U_1 . \quad (18)$$

Here Δ_i is defined as eq. (12) and U_i are fragment excitation energies ($U_2 = U - U_1$), U is the excitation energy of the fissioning compound nuclei and a_i are the level density parameters defined by eq. (6).

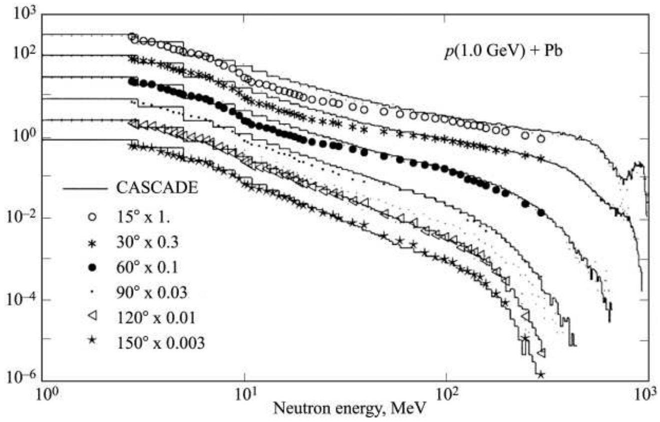

Fig. 1. Energy spectra (mb/MeV/sr) of neutrons created at different angles in the interaction of 1 GeV proton with ^{208}Pb. Experimental points are taken from [44].

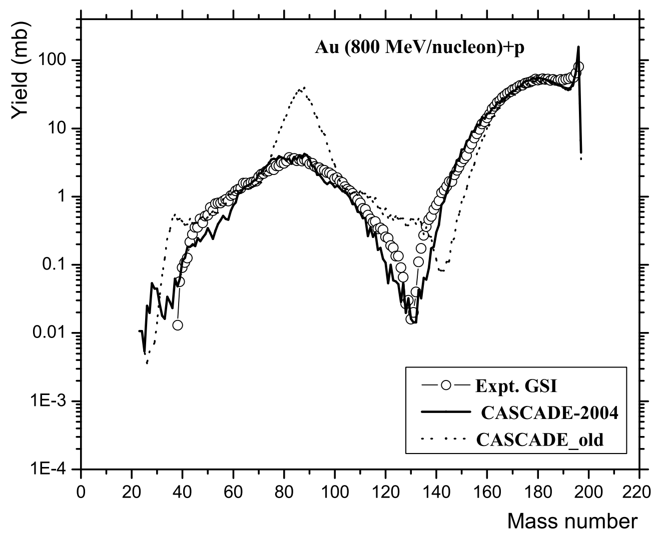

Fig. 2. Mass yield (mb) distribution of isotopes created in inelastic interaction of 0.8 GeV proton with ^{197}Au. Thick and point curves represent calculations by means of the improved version and the old one of the CASCADE code, respectively. Open circles represent experimental data [45,46].

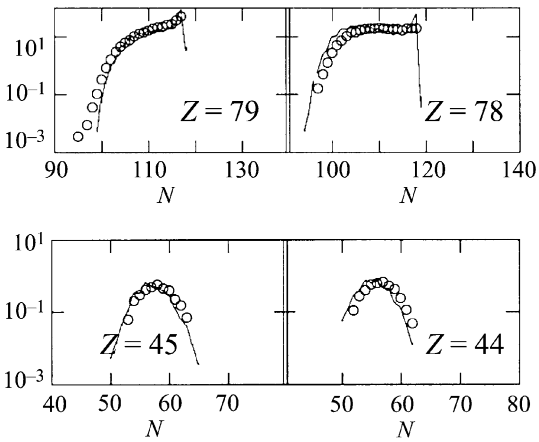

Fig. 3. Yield (mb) distribution of isotopes with charge Z in $p + {}^{197}$Au at $E = 0.8$ GeV. The upper panel shows the spallation yield for $Z = 79$ and 78, the lower one represents the fission yield for $Z = 45$ and 44, N is the number of neutrons. Experimental points are taken from [45,46].

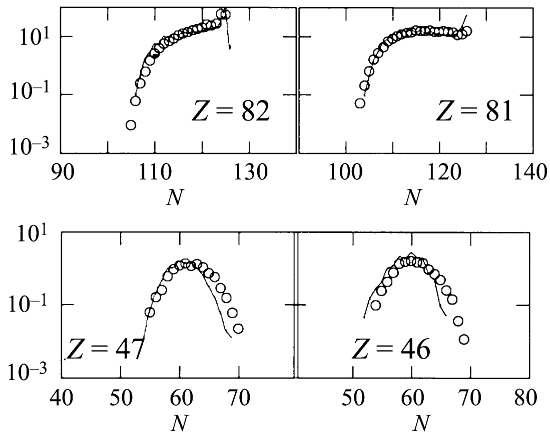

Fig. 5. Yield (mb) distribution of isotopes with charge Z in $p + {}^{208}$Pb at $E = 1$ GeV. The upper panel shows the spallation yield for $Z = 82$ and 81, the lower one represents the fission yield for $Z = 47$ and 46, N is the number of neutrons. Experimental points are taken from [47].

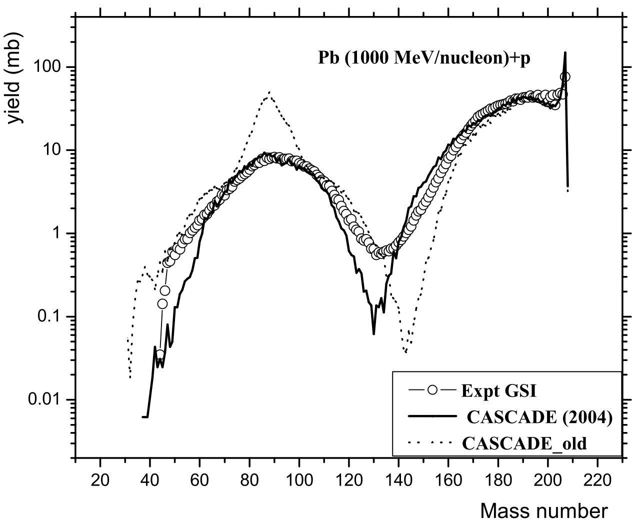

Fig. 4. Mass yield (mb) distribution of isotopes created in inelastic interaction of 1 GeV proton with ^{208}Pb. Notations are similar to those in fig. 2. Experimental data are taken from [47].

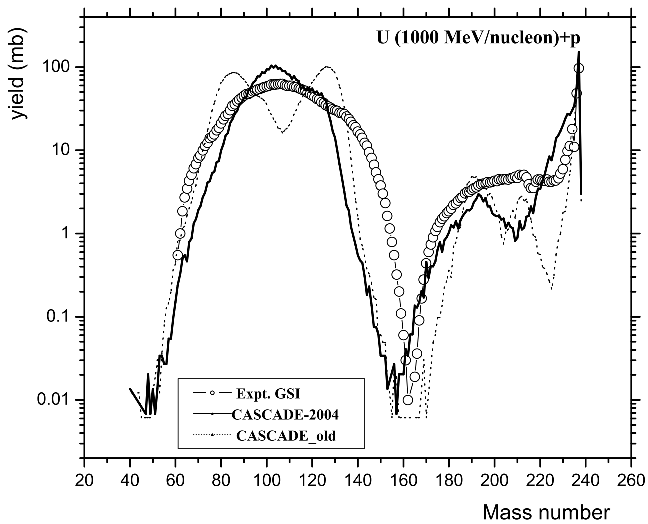

Fig. 6. Mass yield (mb) distribution of isotopes created in the inelastic interaction of 1 GeV proton with ^{238}U. Notations are the same as in fig. 2. Experimental data are taken from [48].

4 Comparison with experiment

The calculated neutron yield, differential and integral spectra of neutrons, are close to the values obtained by means of the previous version of our code and agree with experiment. This can be seen from tables 1, 2 and fig. 1, where, as an example, some data for lead and uranium are presented. The above-described improvements practically do not change the distribution of the produced heat in the target. In the previous version of CASCADE, we had a problem with the calculation of isotope cross-sections. In many cases the experimental and theoretical data differ by a factor of order. The calculated cross-sections are changed significantly by the introduced improvements. This is illustrated by figs. 2-7. In both regions, at the hump created by fission fragments and in the evaporation branch, the agreement with experiment becomes much better, although it is true that some deviations yet remain. For example, in case of uranium the yield of isotopes with mass numbers $A \simeq 140$–160 is essentially less than the experimental one. There are some disagreements for light isotopes. The deviations preserve, as can be seen from fig. 8, even if we take into account the evaporation of heavy fragments. In this region theory needs further development.

5 Conclusions

After the improvements of physical models describing the decay, evaporation and fission, of highly excited residual nuclei, the programme complex CASCADE-2004 can be used for the calculation of the yields, spectral angular distributions of neutron and charged particles created in hadron- and nucleus-nucleus interactions at energies from

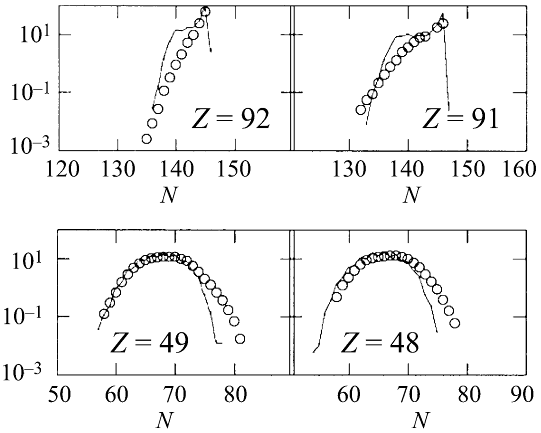

Fig. 7. Yield (mb) distribution of isotopes with charge Z in $p + {}^{238}\mathrm{U}$ at $E = 1$ GeV. The upper panel shows the spallation yield for $Z = 92$ and 91, the lower one represents the fission yield for $Z = 49$ and 48, N is the number of neutrons. Experimental points are taken from [48].

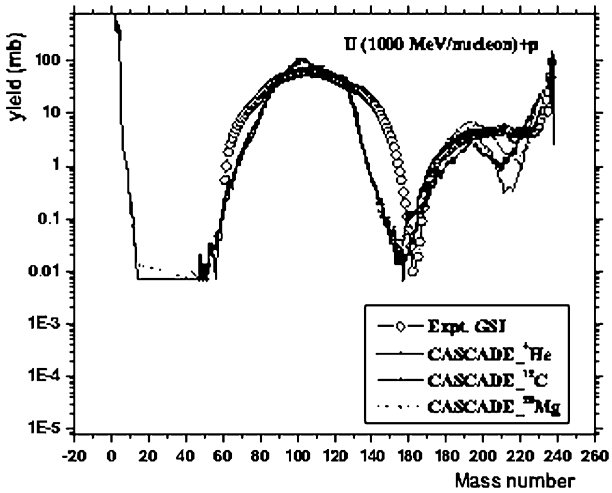

Fig. 8. Calculated isotope mass yield (mb) distribution in the collision of 1 GeV proton with ^{238}U at various numbers of the evaporating particles. Thick curve only six evaporating particles including ^{4}He; thin curve all particles and fragments taken into account including ^{16}C; dotted curve represents particles up to 28_{Mg}. Points represent the experimental data [48].

several tens of MeV up to several tens of GeV and for Monte Carlo modelling of the transport of such particles in matter. The code allows one to consider heterogeneous targets with complicated chemical contents. For a better agreement with experiment, one must improve models of decay of highly excited light nuclei and strong asymmetric fission, which are responsible for light-isotope production.

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