1 MCNP6 fragmentation of light nuclei at intermediate 2 energies

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6 Abstract

Fragmentation reactions induced on light target nuclei by protons and light nuclei of energies around 1 GeV/nucleon and below are studied with the latest Los Alamos Monte Carlo transport code MCNP6 and with its cascade-exciton model (CEM) and Los Alamos version of the quark-gluon string model (LAQGSM) event generators, version 03.03, used as stand-alone codes. Such reactions are involved in different applications, like cosmic-ray-induced single event upsets (SEU's), radiation protection, and cancer therapy with proton and ion beams, among others; therefore, it is important that MCNP6 simulates them as well as possible. CEM and LAQGSM assume that intermediate-energy fragmentation reactions on light nuclei occur generally in two stages. The first stage is the intranuclear cascade (INC), followed by the second, Fermi breakup disintegration of light excited residual nuclei produced after the INC. Both CEM and LAQGSM account also for coalescence of light fragments (complex particles) up to ⁴He from energetic nucleons emitted during INC. We investigate the validity and performance of MCNP6, CEM, and LAQGSM in simulating fragmentation reactions at intermediate energies and discuss possible ways of further improving these codes.

7 *Keywords:* Monte Carlo, transport codes, MCNP6, cascade-exciton model
8 (CEM), Los Alamos version of the quark-gluon string model (LAQGSM),
9 fragmentation, Fermi breakup, coalescence, fragment spectra, production
10 cross-sections

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11 1. Introduction

12 Fragmentation reactions induced by protons and light nuclei of energies
13 around 1 GeV/nucleon and below on light target nuclei are involved in differ-
14 ent applications, like cosmic-ray-induced single event upsets (SEU's), radiation
15 protection, and cancer therapy with proton and ion beams, among others. It is
16 impossible to measure all nuclear data needed for such applications; therefore,
17 Monte Carlo transport codes are usually used to simulate impacts associated
18 with fragmentation reactions. It is important that available transport codes sim-
19 ulate such reactions as well as possible. For this reason, during the past several
20 years, efforts have been done to investigate the validity and performance of, and
21 to improve where possible, nuclear reaction models simulating fragmentation of
22 light nuclei in GEANT4 [1], SHIELD-HIT [2]–[4], and PHITS [5, 6].

23 The Los Alamos Monte Carlo transport code MCNP6 [7] uses the latest
24 version of the cascade-exciton model (CEM) as incorporated in its event gener-
25 ator CEM03.03 [8, 9] to simulate fragmentation of light nuclei at intermediate
26 energies for reactions induced by nucleons, pions, and photons, and the Los
27 Alamos version of the quark-gluon string model (LAQGSM) as implemented in
28 the code LAQGSM03.03 [9, 10] to simulate fragmentation reactions induced by
29 nuclei and by particles at energies above ~ 3.5 GeV, up to about 1 TeV/nucleon
30 (see details in Ref. [7]).

31 In recent years, MCNP6, with its CEM and LAQGSM event generators,
32 has been extensively validated and verified (V&V) against a large variety of
33 nuclear reactions on both thin and thick targets (see, e.g. Refs. [11]–[14] and
34 references therein), but was never tested specifically on fragmentation of light
35 nuclei at intermediate energies. To address this, we investigate the performance
36 of MCNP6, CEM, and LAQGSM in simulating fragmentation reactions at in-
37 termediate energies (from 10 MeV to 5 GeV per nucleon) and discuss possible
38 ways of further improving these codes.

39 2. A Brief Survey of CEM and LAQGSM Physics

40 Details, examples of results, and useful references to different versions of
41 CEM and LAQGSM may be found in a recent lecture [9].

42 The Cascade-Exciton Model (CEM) of nuclear reactions was proposed more
43 than 30 years ago at the Laboratory of Theoretical Physics, JINR, Dubna, USSR
44 by Gudima, Mashnik, and Toneev [15]. It is based on the standard (non-time-
45 dependent) Dubna IntraNuclear Cascade (INC) [16, 17] and the Modified Exci-
46 ton Model (MEM) [18, 19]. The code LAQGSM03.03 is the latest modification
47 [10] of LAQGSM [20], which in its turn is an improvement of the Quark-Gluon
48 String Model (QGSM) [21]. It describes reactions induced by both particles and
49 nuclei at incident energies up to about 1 TeV/nucleon.

50 The basic version of both the CEM and LAQGSM event generators is the
51 so-called “03.03” version, namely CEM03.03 [8, 9, 22] and LAQGSM03.03 [9,
52 10, 23]. The CEM code calculates nuclear reactions induced by nucleons, pions,
53 and photons. It assumes that the reactions occur generally in three stages (see
54 Fig. 1). The first stage is the INC, in which primary particles can be re-scattered
55 and produce secondary particles several times prior to absorption by, or escape
56 from the nucleus. When the cascade stage of a reaction is completed, CEM uses
57 the coalescence model to “create” high-energy d, t, ^3He , and ^4He by final-state
58 interactions among emitted cascade nucleons outside of the target. The emission
59 of the cascade particles determines the particle-hole configuration, Z , A , and the
60 excitation energy that is the starting point for the second, preequilibrium stage
61 of the reaction. The subsequent relaxation of the nuclear excitation is treated
62 in terms of an improved version of the modified exciton model of preequilibrium
63 decay followed by the equilibrium evaporation/fission stage.

64 Generally, all three components may contribute to experimentally measured
65 particle spectra and other distributions. But if the residual nuclei after the
66 INC have mass numbers with $A \leq A_{Fermi} = 12$, CEM uses the Fermi breakup
67 model to calculate their further disintegration instead of using the preequilib-
68 rium and evaporation models. Fermi breakup is much faster to calculate and

Figure 1: Flow chart of nuclear-reaction calculations by CEM03.03 and LAQGSM03.03.

69 gives results very similar to the continuation of the more detailed models to
 70 much lighter nuclei. LAQGSM also describes nuclear reactions, generally, as a
 71 three-stage process: INC, followed by preequilibrium emission of particles dur-
 72 ing the equilibration of the excited residual nuclei formed after the INC, followed
 73 by evaporation of particles from or fission of the compound nuclei. LAQGSM
 74 was developed with a primary focus on describing reactions induced by nuclei,
 75 as well as induced by most elementary particles (see details in Ref. [20]), at
 76 high energies, up to about 1 TeV/nucleon. Although the INC of LAQGSM is
 77 completely different from the one in CEM (see Section 1.1.1), LAQGSM also
 78 considers Fermi breakup of nuclei with $A \leq 12$ produced after the cascade,
 79 and the coalescence model to “produce” high-energy d, t, ^3He , and ^4He from
 80 nucleons emitted during the INC.

81 Many people participated in the CEM and LAQGSM code development over
 82 their more than 40-year history. Current contributors to their “03.03” versions
 83 are S. G. Mashnik, K. K. Gudima, A. J. Sierk, R. E. Prael, M. I. Baznat, and
 84 N. V. Mokhov. One of the authors (L.M.K.) has joined these efforts recently
 85 to extend the preequilibrium models of CEM and LAQGSM by accounting for
 86 possible emission of light fragment (LF) heavier than ^4He , up to ^{28}Mg .

87 2.1. The Intranuclear Cascade Mechanism

88 The INC approach is based on the ideas of Heisenberg and Serber, who re-
89 garded intranuclear cascades as a series of successive quasi-free collisions of the
90 fast primary particle with the individual nucleons of the nucleus. Basic assump-
91 tions of and conditions for INC applicability may be found in [9]. Comprehensive
92 details and useful references are published in [16, 17].

93 2.1.1. The INC of CEM03.03

94 The intranuclear cascade model in CEM03.03 is based on the standard (non-
95 time-dependent) version of the Dubna cascade model [16, 17]. All the cascade
96 calculations are carried out in a three-dimensional geometry. The nuclear matter
97 density $\rho(r)$ is described by a Fermi distribution with two parameters taken from
98 the analysis of electron-nucleus scattering. For simplicity, the target nucleus is
99 divided by concentric spheres into seven zones in which the nuclear density is
100 considered to be constant. The energy spectrum of the target nucleons is es-
101 timated in the perfect Fermi-gas approximation. The influence of intranuclear
102 nucleons on the incoming projectile is taken into account by adding to its lab-
103 oratory kinetic energy an effective real potential, as well as by considering the
104 Pauli principle which forbids a number of intranuclear collisions and effectively
105 increases the mean free path of cascade particles inside the target. The inter-
106 action of the incident particle with the nucleus is approximated as a series of
107 successive quasi-free collisions of the fast cascade particles (N , π , or γ) with
108 intranuclear nucleons.

109 The integral cross sections for the free NN , πN , and γN interactions are
110 approximated in the Dubna INC model [16, 17] using a special algorithm of
111 interpolation/extrapolation through a number of picked points, mapping as well
112 as possible the experimental data. This was done very accurately by Prof.
113 Barashenkov's group using all experimental data available at that time, more
114 than 45 years ago [24]. Currently the experimental data on cross sections is much
115 more complete than at that time; therefore we have revised the approximations
116 of all the integral elementary cross sections used in CEM.

117 The kinematics of two-body elementary interactions and absorption of pho-
 118 tons and pions by a pair of nucleons is completely defined by a given direction
 119 of emission of one of the secondary particles. The cosine of the angle of emission
 120 of secondary particles in the c.m. system is calculated by the Dubna INC with
 121 approximations based on available experimental data. For elementary interac-
 122 tions with more than two particles in the final state, the Dubna INC uses the
 123 statistical model to simulate the angles and energies of products (see details in
 124 [16]).

125 For the improved version of the INC in CEM03.03, we use currently available
 126 experimental data and recently published systematics proposed by other authors
 127 and have developed new approximations for angular and energy distributions of
 128 particles produced in nucleon-nucleon and photon-proton interactions. In addi-
 129 tion, we have incorporated into newer versions of CEM a possibility to normalize
 130 the final results to systematics based on available experimental reaction cross
 131 sections. The condition for the transition from the INC stage of a reaction to
 132 preequilibrium was changed; on the whole, the INC stage in CEM03.03 is longer
 133 while the preequilibrium stage is shorter in comparison with previous versions.
 134 We have incorporated real binding energies for nucleons in the cascade instead
 135 of the approximation of a constant separation energy of 7 MeV used in the
 136 initial versions of the CEM and have imposed momentum-energy conservation
 137 for each simulated event (conservation was only “on the average” in earlier ver-
 138 sions). Along with the improved elementary cross sections, we also changed and
 139 improved the algorithms of many INC routines and many INC routines were
 140 rewritten, which significantly speeded up the code. Details, examples of results,
 141 and references to this portion of our work may be found in [9].

142 2.1.2. *The INC of LAQGSM03.03*

143 The INC of LAQGSM03.03 is described with a recently improved version
 144 [10, 23, 25] of the time-dependent intranuclear cascade model developed initially
 145 at JINR in Dubna, often referred to in the literature as the Dubna intranuclear
 146 Cascade Model, DCM (see [26] and references therein). The DCM models in-

147 teractions of fast cascade particles (“participants”) with nucleon spectators of
148 both the target and projectile nuclei and includes as well interactions of two
149 participants (cascade particles). It uses experimental cross sections at ener-
150 gies below 4.5 GeV/nucleon, and those calculated by the Quark-Gluon String
151 Model [21, 27] at higher energies to simulate angular and energy distributions
152 of cascade particles, and also considers the Pauli Exclusion Principle.

153 In contrast to the CEM version of the INC described above, DCM uses a
154 continuous nuclear density distribution; therefore, it does not need to consider
155 refraction and reflection of cascade particles inside or on the border of a nucleus.
156 It also keeps track of the time of an intranuclear collision and of the depletion
157 of the nuclear density during the development of the cascade (the so-called
158 “trawling effect”) and takes into account the hadron formation time.

159 All the new approximations developed recently for the INC of CEM to de-
160 scribe total cross sections and elementary energy and angular distributions of
161 secondary particles from hadron-hadron interactions have been incorporated
162 also into the INC of LAQGSM [23]. In addition, a new high-energy photonuc-
163 clear reaction model based on the event generators for γp and γn reactions from
164 the Moscow INC [28] (kindly provided to us by Dr. Igor Pshenichnov) and on
165 the latest photonuclear version of CEM [29] was developed and incorporated into
166 the INC of LAQGSM; this allows us to calculate reactions induced by photons
167 with energies of up to tens of GeV. In the latest version of LAQGSM [10], the
168 INC was modified for a better description of nuclear reactions at very high en-
169 ergies (above 20 GeV/nucleon). Finally, the algorithms of many LAQGSM INC
170 routines were revised and some INC routines were rewritten, which speeded up
171 the code significantly. Details, examples of results, and references to this portion
172 of our work may be found in [9].

173 *2.2. The Coalescence Model*

174 When the cascade stage of a reaction is completed, CEM and LAQGSM use
175 the coalescence model described in Ref. [26] to “create” high-energy d, t, ^3He ,
176 and ^4He by final-state interactions among emitted cascade nucleons outside of

177 the target nucleus. In contrast to most other coalescence models for heavy-
 178 ion-induced reactions, where complex-particle spectra are estimated simply by
 179 convolving the measured or calculated inclusive spectra of nucleons with corre-
 180 sponding fitted coefficients, CEM03.03 and LAQGSM03.03 use in their simula-
 181 tions of particle coalescence real information about all emitted cascade nucleons
 182 and do not use integrated spectra. We assume that all the cascade nucleons
 183 having differences in their momenta smaller than p_c and the correct isotopic
 184 content form an appropriate composite particle. The coalescence radii p_c were
 185 fitted for each composite particle in Ref. [26] to describe available data for the
 186 reaction Ne+U at 1.04 GeV/nucleon. The fitted values turned out to be quite
 187 universal and were subsequently found to describe high-energy complex-particle
 188 production satisfactorily for a variety of reactions induced both by particles and
 189 nuclei at incident energies up to about 200 GeV/nucleon, when describing nu-
 190 clear reactions with different versions of LAQGSM [9] or with its predecessor,
 191 the Quark-Gluon String Model (QGSM) [21]. These parameters are:

$$\begin{aligned}
 p_c(d) &= 90 \text{ MeV/c} ; \\
 p_c(t) &= p_c(^3\text{He}) = 108 \text{ MeV/c} ; \\
 p_c(^4\text{He}) &= 115 \text{ MeV/c} .
 \end{aligned}
 \tag{1}$$

192 As the INC of CEM is different from those of LAQGSM or QGSM, it is
 193 natural to expect different best values for p_c as well. Our recent studies show
 194 that the values of parameters p_c defined by Eq. (1) are also good for CEM for
 195 projectile particles with kinetic energies T_0 lower than 300 MeV and equal to
 196 or above 1 GeV. For incident energies in the interval $300 \text{ MeV} \leq T_0 < 1 \text{ GeV}$,
 197 a better overall agreement with the available experimental data is obtained
 198 by using values of p_c equal to 150, 175, and 175 MeV/c for d, t (^3He), and
 199 ^4He , respectively. These values of p_c are fixed as defaults in CEM03.03. If
 200 several cascade nucleons are chosen to coalesce into composite particles, they
 201 are removed from the distributions of nucleons and do not contribute further to
 202 such nucleon characteristics as spectra, multiplicities, *etc.*

203 In comparison with the initial version [26], in CEM03.03 and LAQGSM03.03,

several coalescence routines have been changed/deleted and have been tested against a large variety of measured data on nucleon- and nucleus-induced reactions at different incident energies.

2.3. Preequilibrium Reactions

The subsequent preequilibrium interaction stage of nuclear reactions is considered by our current CEM and LAQGSM in the framework of the latest version of the Modified Exciton Model (MEM) [18, 19] as described in Ref. [22]. At the preequilibrium stage of a reaction, we take into account all possible nuclear transitions changing the number of excitons n with $\Delta_n = +2, -2$, and 0, as well as all possible multiple subsequent emissions of n, p, d, t, ^3He , and ^4He (see the exact definition of “excitons” we use here in Ref. [15]). The corresponding system of master equations describing the behavior of a nucleus at the preequilibrium stage is solved by the Monte-Carlo technique [15].

CEM considers the possibility of fast d, t, ^3He , and ^4He emission at the preequilibrium stage of a reaction in addition to the emission of nucleons. We assume that in the course of a reaction p_j excited nucleons (excitons) are able to condense with probability γ_j forming a complex particle which can be emitted during the preequilibrium state. The “condensation” probability γ_j is estimated as the overlap integral of the wave function of independent nucleons with that of the complex particle (see details in [15])

$$\gamma_j \simeq p_j^3 (V_j/V)^{p_j-1} = p_j^3 (p_j/A)^{p_j-1} . \quad (2)$$

This is a rather crude estimate. As is frequently done, the values γ_j are taken from fitting the theoretical preequilibrium spectra to the experimental ones. In CEM, to improve the description of preequilibrium complex-particle emission, we estimate γ_j by multiplying the estimate provided by Eq. (2) by an empirical coefficient $M_j(A, Z, T_0)$ whose values are fitted to available nucleon-induced experimental complex-particle spectra.

CEM and LAQGSM predict forward-peaked (in the laboratory system) angular distributions for preequilibrium particles. For instance, CEM assumes that

232 a nuclear state with a given excitation energy E^* should be specified not only by
 233 the exciton number n but also by the momentum direction Ω . This calculation
 234 scheme is easily realized by the Monte-Carlo technique [15]. It provides a good
 235 description of double differential spectra of preequilibrium nucleons and a not-
 236 so-good but still satisfactory description of complex-particle spectra from differ-
 237 ent types of nuclear reactions at incident energies from tens of MeV to several
 238 GeV. For incident energies below about 200 MeV, Kalbach [30] has developed a
 239 phenomenological systematics for preequilibrium-particle angular distributions
 240 by fitting available measured spectra of nucleons and complex particles. As the
 241 Kalbach systematics are based on measured spectra, they describe very well
 242 the double-differential spectra of preequilibrium particles and generally provide
 243 a better agreement of calculated preequilibrium complex-particle spectra with
 244 data than does the CEM approach [15]. This is why we have incorporated into
 245 CEM03.03 and LAQGSM03.03 the Kalbach systematics [30] to describe angular
 246 distributions of both preequilibrium nucleons and complex particles at incident
 247 energies up to 210 MeV. At higher energies, we use the CEM approach [15].

248 The standard version of the CEM [15] provides an overestimation of preequi-
 249 librium particle emission from different reactions we have analyzed (see more
 250 details in [31]). One way to solve this problem, suggested in Ref. [31], is to
 251 change the criterion for the transition from the cascade stage to the preequi-
 252 librium one. Another easy way, suggested in Ref. [31], to shorten the preequi-
 253 librium stage of a reaction is to arbitrarily allow only transitions that increase
 254 the number of excitons, $\Delta n = +2$, *i.e.*, only allow the evolution of a nucleus
 255 toward the compound nucleus. In this case, the time of the equilibration will
 256 be shorter and fewer preequilibrium particles will be emitted, leaving more ex-
 257 citation energy for the evaporation. This approach was used in the CEM2k [31]
 258 version of the CEM and it allowed us to describe much better the p+A reac-
 259 tions measured at GSI in inverse kinematics at energies around 1 GeV/nucleon.
 260 Nevertheless, the “never-come-back” approach seems unphysical; therefore we
 261 no longer use it. We now address the problem of emitting fewer preequilibrium
 262 particles in the CEM by following Veselsky [32]. We assume that the ratio of

the number of quasi-particles (excitons) n at each preequilibrium reaction stage to the number of excitons in the equilibrium configuration n_{eq} , corresponding to the same excitation energy, to be a crucial parameter for determining the probability of preequilibrium emission P_{pre} (see details in [9, 22, 32]). Algorithms of many preequilibrium routines were changed and almost all these routines were rewritten, which has speeded up the code significantly relative to earlier versions [9, 22].

2.4. Evaporation

CEM and LAQGSM use an extension of the Generalized Evaporation Model (GEM) code GEM2 by Furihata [33] after the preequilibrium stage of reactions to describe evaporation of nucleons, complex particles, and light fragments heavier than ${}^4\text{He}$ (up to ${}^{28}\text{Mg}$) from excited compound nuclei and to describe fission, if the compound nuclei are heavy enough to fission ($Z \geq 65$).

When including evaporation of up to 66 types of particles in GEM2, running times increase significantly compared to the case when evaporating only 6 types of particles, up to ${}^4\text{He}$. The major particles emitted from an excited nucleus are n, p, d, t, ${}^3\text{He}$, and ${}^4\text{He}$. For most cases, the total emission probability of particles heavier than α is negligible compared to those for the emission of light ejectiles. Our detailed investigation of different reactions shows that if we study only nucleon and complex-particle spectra or only spallation and fission products and are not interested in light fragments, we can consider evaporation of only 6 types of particles in GEM2 and save much time, getting results very close to the ones calculated with the more time consuming “66” option. In our current code versions, we allow the number of types of evaporated particles to be selected in advance. A detailed description of GEM2, as incorporated into CEM and LAQGSM, may be found in [9, 22].

2.5. Fission

The fission model used in GEM2 is based on Atchison’s model [34], often referred to in the literature as the Rutherford Appleton Laboratory (RAL) fission

model, which is where Atchison developed it. The mass-, charge-, and kinetic energy-distribution of fission fragments are simulated by RAL using approximations based on available experimental data (see details in [9, 22, 33, 34]). For CEM03.03 and LAQGSM03.03, we modified slightly [35] GEM2. Since in this study we consider only reactions on light, not fissioning nuclei, we will not discuss further the fission model; interested readers may find details and further references in [9, 22, 35, 36].

2.6. The Fermi Breakup Model

After calculating the coalescence stage of a reaction, CEM and LAQGSM move to the description of the last slow stages of the interaction, namely to preequilibrium decay and evaporation, with a possible competition of fission. But at any stage, if the residual nuclei have mass numbers with $A \leq A_{Fermi} = 12$, CEM and LAQGSM use the Fermi breakup model [37] to calculate their further disintegration instead of using the preequilibrium and evaporation models. All formulas and details of the algorithms used in the version of the Fermi breakup model developed in the group of the Late Prof. Barashenkov at JINR, Dubna, may be found in [38]; we use this model.

The original version of the model contained a few features which very occasionally could lead to unphysical fragments; these could cause problems in a transport model. All these issues have been dealt with in the current version, which no longer encounters such problems.

As described above, de-excitation of light nuclei with $A \leq A_{Fermi}$ produced after the INC is described by CEM and LAQGSM only with the Fermi breakup model, where A_{Fermi} is a “cut-off value” fixed in our models. The value of A_{Fermi} is a model dependent parameter, not a physics characteristic of nuclear reactions. Actually, the initial version of the Fermi breakup model we incorporated in CEM and LAQGSM [22, 23] was used when $A \leq A_{Fermi} = 16$, just as $A_{Fermi} = 16$ is used currently in GEANT4 (see [1]) and in SHIELD-HIT (see [2]–[4]). But as mentioned in Section 2.6, that initial version of the Fermi breakup model had some problems and crashed our codes in some cases.

322 To avoid unphysical results and code crashes, we chose the expedient of using
 323 $A_{Fermi} = 12$ in both CEM and LAQGSM. Later, we fixed the problems in the
 324 Fermi break-up model, but did not at that time change the value of A_{Fermi} , and
 325 never studied how its value affects the final results calculated in these codes.

326 3. Results

327 As mentioned in the previous section, we never studied how the value of
 328 A_{Fermi} affects the results of nuclear reactions on light nuclei simulated with
 329 CEM and LAQGSM. We address this here, calculating spectra of emitted par-
 330 ticles and light fragments, and yields of all possible products from various re-
 331 actions using different values for A_{Fermi} . We discuss below separately product
 332 cross sections (Section 3.1) and spectra of particles and light fragments (Section
 333 3.2).

334 3.1. Fragment production cross sections

335 One of the most difficult tasks for any theoretical model is to predict cross
 336 sections of arbitrary products as functions of the incident energy of the pro-
 337 jectiles initiating the reactions, *i.e.*, excitation functions. Therefore, we chose
 338 to start our study with comparing the available experimental data on excita-
 339 tion functions of products from several proton-induced reactions on light nuclei
 340 at intermediate energies with predictions by MCNP6 using its default event
 341 generator for such reactions, CEM03.03, as well as with results calculated by
 342 CEM03.03 used as a stand-alone code.

343 Figs. 2–15 present examples of excitation functions for all products we found
 344 at least several measured values for proton-induced reactions on ^{14}N , ^{16}O , ^{27}Al ,
 345 and ^{28}Si . To understand better the reasons of agreements or disagreements
 346 of calculated values with the measured excitation functions, we present in our
 347 figures also the total reaction cross sections, experimental and theoretical.

348 Figs. 2–5 show our results for the $p + ^{14}\text{N}$ reaction. The first thing to
 349 note is that the total reaction cross sections simulated with MCNP6 and shown

Figure 2: Total inelastic cross section and excitation functions for the production of ^{14}O , ^{13}N , and ^{12}N from $p + ^{14}\text{N}$ calculated with CEM03.03 using the “standard” version of the Fermi breakup model ($A_{\text{Fermi}} = 12$) and with a cut-off value of 16 for A_{Fermi} , as well as with MCNP6 using CEM03.03 ($A_{\text{Fermi}} = 12$) compared with experimental data, as indicated. Experimental data for inelastic cross sections are from Refs. [39]–[41], while the data for excitation functions are from the T16 Lib compilation [42].

350 in the upper-left plot in Fig. 2 with small solid circles agree well with the
 351 available experimental data (symbols) and with calculations by CEM03.03 used
 352 as a stand-alone code (solid line). There is a difference between the models,
 353 especially in the regions of incident proton energies $T_p = 50 - 100$ MeV and
 354 $T_p \geq 2$ GeV. To be expected, since MCNP6 and CEM03.03 use very similar,
 355 but slightly different approximations for the total proton-nucleus reaction cross
 356 sections (see details and references in [7, 8]). These little differences in the
 357 total reaction cross sections will produce, respectively, similar differences in all
 358 excitation functions simulated with MCNP6 and CEM03.03.

Figure 3: Excitation functions for the production of ^{13}C , ^{12}C , ^{11}C , and ^{10}C from $p + ^{14}\text{N}$ calculated with CEM03.03 using the “standard” version of the Fermi breakup model ($A_{\text{Fermi}} = 12$) and with a cut-off value of 16 for A_{Fermi} , as well as with MCNP6 using CEM03.03 ($A_{\text{Fermi}} = 12$) compared with experimental data, as indicated. Experimental data are from the T16 Lib compilation [42].

359 The total reaction cross sections are based on systematics (see details and
 360 references in [7, 8]), therefore they do not depend on the value of A_{Fermi} we
 361 use in our calculations. However, we performed calculations of all excitation
 362 functions shown in Figs. 2 to 5 with CEM03.03 used as a stand-alone code with
 363 its “default value” $A_{\text{Fermi}} = 12$, as well as with a modification of the code using
 364 $A_{\text{Fermi}} = 16$, which in case of these $p + ^{14}\text{N}$ reactions, actually corresponds to
 365 $A_{\text{Fermi}} = 14$. We cannot get a mass number $A = 16$ from $p + ^{14}\text{N}$ interactions,
 366 and even a nucleus with $A = 15$ would not be produced by the INC of CEM03.03
 367 at these intermediate energies.

368 First, from the results presented in Figs. 2 to 5, we see a very good agreement

Figure 4: The same as in Fig. 3, but for the production of ^{11}B , ^{10}B , ^{10}Be , and ^9Be .

369 between the excitation functions simulated by MCNP6 using CEM03.03 and cal-
 370 culations by CEM03.03 used as a stand-alone code, and a reasonable agreement
 371 with most available experimental data. This fact serves as a validation and ver-
 372 ification (V&V) of MCNP6 and shows no problems with the implementation of
 373 CEM03.03 in MCNP6 or with the simulations of these reactions by either code.

374 Second, we'd like to explicitly inform the readers that we do not worry too
 375 much about some observed discrepancies between some calculated excitation
 376 functions and measured data at low energies, below 20 MeV. As the default,
 377 MCNP6 uses data libraries at such low energies and never uses CEM03.03 or
 378 its other event generators, if data libraries are available (MCNP6 has proton-
 379 induced data libraries for the reactions studied here). By contrast, CEM uses its
 380 INC to simulate the first stage of nuclear reactions, and the INC is not supposed
 381 to work properly at such low energies (see details in [8, 9]).

Figure 5: The same as in Fig. 3, but for the production of ${}^7\text{Be}$, ${}^9\text{Li}$, ${}^8\text{Li}$, and t .

382 Third, results calculated both with $A_{Fermi} = 12$ and 16 agree reasonably
 383 well with available data, taking into account that all calculations, at all energies
 384 and for all reactions were done with the fixed version of our codes, without any
 385 tuning or changing of any parameters. However, in some cases, we can observe
 386 significant differences between excitation functions calculated with $A_{Fermi} = 12$
 387 and 16.

388 For this particular reaction, the excitation functions for the production of
 389 ${}^{14}\text{O}$, ${}^{13}\text{N}$, ${}^{12}\text{N}$, ${}^{13}\text{C}$, ${}^{12}\text{C}$, and ${}^{10}\text{C}$ calculated with $A_{Fermi} = 16$ (that for our p
 390 + ${}^{14}\text{N}$ reaction is the same as $A_{Fermi} = 14$, which from a physical point of view
 391 means that we use only Fermi breakup after INC and never use preequilibrium
 392 and/or evaporation models to calculate this reaction) agree better with available
 393 experimental data than results obtained with $A_{Fermi} = 12$. On the other hand,
 394 excitation functions for the production of ${}^9\text{Be}$ and ${}^7\text{Be}$ are reproduced better

Figure 6: Total inelastic cross section and excitation functions for the production of ^{15}O , ^{14}O , and ^{13}N from $p + ^{16}\text{O}$ calculated with CEM03.03 using the “standard” version of the Fermi breakup model ($A_{\text{Fermi}} = 12$) and with cut-off values for A_{Fermi} of 16 and 14, as well as with MCNP6 using CEM03.03 ($A_{\text{Fermi}} = 12$) compared with experimental data, as indicated. Experimental data for inelastic cross sections are from Refs. [39, 43, 44], while the data for excitation functions are from the T16 Lib compilation [42].

395 with $A_{\text{Fermi}} = 12$.

396 Figs. 6 to 9 present results similar to the ones shown in Figs. 2 to 5, but
 397 for the reaction $p + ^{16}\text{O}$. Most of the experimental data for these reactions
 398 were measured on ^{nat}O , with only a few data points obtained for ^{16}O ; all our
 399 calculations were performed for ^{16}O . For these reactions, we performed three
 400 sets of calculations, using $A_{\text{Fermi}} = 12$, 14, and 16 in CEM03.03. The general
 401 agreement/disagreement of our results with available measured data for oxygen
 402 is very similar to what we showed above for $p + ^{14}\text{N}$, with the major difference
 403 that almost all products from oxygen are better predicted with $A_{\text{Fermi}} = 14$;

Figure 7: Excitation functions for the production of ^{14}C , ^{11}C , ^{10}C , and ^{11}B from $p + ^{16}\text{O}$ calculated with CEM03.03 using the “standard” version of the Fermi breakup model ($A_{\text{Fermi}} = 12$) and with cut-off values for A_{Fermi} of 16 and 14, as well as with MCNP6 using CEM03.03 ($A_{\text{Fermi}} = 12$) compared with experimental data, as indicated. Experimental data are from the T16 Lib compilation [42].

404 production of ^{11}B is described a little better with $A_{\text{Fermi}} = 16$, while ^9Be and
 405 ^7Be are reproduced better with $A_{\text{Fermi}} = 12$, just as for nitrogen (see Figs. 4
 406 and 5).

407 Figs. 10 to 15 show results similar to those in Figs. 2–9, but for proton
 408 interactions with ^{27}Al and ^{28}Si . All reactions on silicon were calculated for ^{28}Si ,
 409 while most of the data were measured from ^{nat}Si (see details in legends of Fig.
 410 14). Aluminum and silicon are interesting because they are used in many ap-
 411 plications. From a theoretical point of view, $p + ^{27}\text{Al}$ and ^{28}Si reactions are
 412 challenging because Al and Si are relatively light, with significant contributions
 413 from the Fermi breakup models in our simulations. At the same time Al and

Figure 8: The same as in Fig. 7, but for the production of ^{10}B , ^{10}Be , ^9Be , and ^7Be .

414 Si have mass numbers higher than the cut-off discussed above, allowing some
 415 significant contribution to the calculated values from preequilibrium and evap-
 416 oration processes. On the whole, the agreement of the results with available
 417 measured data for Al and Si is very similar to what we find for N and O.

418 In many cases, we get a better description of the heavy fragments when we
 419 use $A_{Fermi} = 16$ or 14 , and usually we predict a little better the light fragments
 420 using $A_{Fermi} = 12$. For comparison, for Al and Si, we show also excitation
 421 functions for the production of all complex particles from d to ^4He , as well as
 422 of secondary protons, as we found experimental data available for them (see
 423 Figs. 11, 12, 14, and 15). Because the absolute values of the yields of light
 424 fragment production is much lower compared to the yields of complex particles,
 425 and especially of protons, the production cross sections of d, t, ^3He , ^4He , and
 426 especially of p calculated with different values of A_{Fermi} are very close to each

Figure 9: The same as in Fig. 7, but for the production of ${}^9\text{Li}$, ${}^7\text{Li}$, ${}^6\text{Li}$, and t .

427 other. This is true also for the production of neutrons; although we do not
 428 have experimental data for neutron production for these reactions. Generally,
 429 emission of nucleons and complex particles are the most determinative in the
 430 calculation of spallation products (heavier residuals) from reactions on medium-
 431 mass nuclei, while LF yields are generally low, and their calculation does not
 432 affect significantly the final cross sections for these heavier products.

433 Figs. 16 and 17 show mass-number dependences of the yield of H, He, Li,
 434 Be, B, C, N, and O isotopes produced in 600 MeV $p + {}^{16}\text{O}$, with a comparison
 435 of our CEM results calculated with $A_{Fermi} = 12$ and 16 with measured data
 436 from Ref. [47]. There is a relatively good agreement of both values of A_{Fermi} ,
 437 which does not allow us to choose a preferred value. The yields of ${}^{11}\text{B}$, ${}^{12}\text{B}$, and
 438 ${}^{14}\text{O}$ with $A_{Fermi} = 16$ agree better with the data, while that of ${}^{12}\text{N}$ is predicted
 439 better using $A_{Fermi} = 12$.

Figure 10: Total inelastic cross section and excitation functions for the production of ^{13}N , ^{11}C , and ^{10}Be , from $p + ^{27}\text{Al}$ calculated with CEM03.03 using the “standard” version of the Fermi breakup model ($A_{\text{Fermi}} = 12$) and with cut-off values for A_{Fermi} of 16 and 14, as well as with MCNP6 using CEM03.03 ($A_{\text{Fermi}} = 12$) compared with experimental data, as indicated. Experimental data for inelastic cross sections are from Refs. [39, 45, 46], while the data for excitation functions are from the T16 Lib compilation [42].

440 Fig. 18 shows an example of one more type of nuclear reaction charac-
 441 teristic: Atomic-number dependence of the fragment-production cross sections
 442 from the interactions of ^{20}Ne (600 MeV/nucleon) with H. For this reaction, be-
 443 sides experimental data from Ref. [49], we compare to results calculated with
 444 CEM03.03 used as a stand-alone code with $A_{\text{Fermi}} = 12$ and 16, results by
 445 MCNP6 using the CEM03.03 event generator with $A_{\text{Fermi}} = 12$, as well as re-
 446 sults by the NASA semi-empirical nuclear fragmentation code NUCFRG2 [50],
 447 and by a parameterization by Nilsen et al. [51] taken from Tab. III of Ref. [49].
 448 We see that all models agree quite well with the measured data, especially

Figure 11: Excitation functions for the production of ${}^7\text{Be}$, ${}^9\text{Li}$, ${}^6\text{He}$, and ${}^4\text{He}$ from $p + {}^{27}\text{Al}$ calculated with CEM03.03 using the “standard” version of the Fermi breakup model ($A_{\text{Fermi}} = 12$) and with cut-off values for A_{Fermi} of 16 and 14, as well as with MCNP6 using CEM03.03 ($A_{\text{Fermi}} = 12$) compared with experimental data, as indicated. Experimental data are from the T16 Lib compilation [42].

449 for LF with $Z > 4$. For LF with $Z > 4$, it is difficult to determine from
 450 which version of CEM03.03 results agree better with the data: the one using
 451 $A_{\text{Fermi}} = 12$ or the one with $A_{\text{Fermi}} = 16$. Light fragments with $Z = 3$ and
 452 4 are described a little better with the $A_{\text{Fermi}} = 12$ version. As we discuss at
 453 the end of the next Section, preequilibrium emission described with an extended
 454 version of the CEM (not accounted for in our calculations shown in Fig. 18), can
 455 be important and may change the final CEM results for this reaction; therefore
 456 we are not ready to make a final decision about which version of the Fermi
 457 breakup model works better for this system.

458 All the examples in Figs. 2 to 18 are for reactions induced by protons, which

Figure 12: The same as in Fig. 11, but for the production of ^3He , t , d , and p .

459 at such relatively low incident energies are simulated by default in MCNP6 with
 460 CEM03.03. Figs. 19 and 20 show examples of nucleus-nucleus reactions with
 461 light nuclei, *i.e.*, involving the Fermi breakup model, but simulated in MCNP6
 462 with LAQGSM03.03. The figures compare experimental [48, 49] Z -dependences
 463 of products from interactions of 290 MeV/nucleon ^{14}Ne and ^{16}O with C and
 464 Al; 600 MeV/nucleon ^{20}Ne with C and Al; and 400 MeV/nucleon ^{24}Mg with
 465 C and Al with LAQGSM03.03 results using $A_{\text{Fermi}} = 12$ and 16, as well as
 466 with results of calculations using models of Refs. [50–52], in the case of 600
 467 MeV/nucleon $^{20}\text{Ne} + \text{C}$ and Al.

468 The cross sections shown in Figs. 19 and 20 are only for the fragmentation
 469 of the projectile-nuclei ^{14}N , ^{16}O , ^{20}Ne , and ^{24}Mg ; they do not contain contribu-
 470 tions from the fragmentation of the C and Al target-nuclei. For all calculations
 471 using all models general agreement to the experimental data is quite good. On

Figure 13: Total inelastic cross section and excitation functions for the production of ^{13}N , ^{14}C , and ^{11}C , from $p + ^{28}\text{Si}$ calculated with CEM03.03 using the “standard” version of the Fermi breakup model ($A_{\text{Fermi}} = 12$) and with cut-off values for A_{Fermi} of 16 and 14, as well as with MCNP6 using CEM03.03 ($A_{\text{Fermi}} = 12$) compared with experimental data, as indicated. Experimental data for inelastic cross sections are from Refs. [39, 45], while the data for excitation functions are from the T16 Lib compilation [42].

the whole, for these particular reactions, the products with $Z = 3$ and 4 are described a little better with the $A_{\text{Fermi}} = 12$ version of LAQGSM, while heavier fragments are often predicted better with $A_{\text{Fermi}} = 16$.

3.2. Fragment spectra

This Section presents several examples of particle and LF spectra from various proton- and nucleus-induced reactions, chosen so that although all of them are fragmentation of light nuclei at intermediate energies, they address different reaction mechanisms of fragment production, sometimes involving several mechanisms in the production of the same LF in a given reaction.

Figure 14: Excitation functions for the production of ^{10}Be , ^7Be , ^9Li , and ^4He from $p + ^{28}\text{Si}$ calculated with CEM03.03 using the “standard” version of the Fermi breakup model ($A_{\text{Fermi}} = 12$) and with cut-off values for A_{Fermi} of 16 and 14, as well as with MCNP6 using CEM03.03 ($A_{\text{Fermi}} = 12$) compared with experimental data, as indicated. Experimental data are from the T16 Lib compilation [42].

481 Figs. 21 to 23 show examples of measured particle and LF double-differential
 482 spectra from $p + ^9\text{Be}$ at 190 and 300 MeV [53], as well as at 392 MeV [54]
 483 (symbols) compared with our CEM results (histograms). Because ^9Be has a
 484 mass number $A < A_{\text{Fermi}} = 12$, all the LF from these reactions are calculated by
 485 CEM either as fragments from the Fermi breakup of the excited nuclei remaining
 486 after the initial INC stage of reactions, or as “residual nuclei” after emission
 487 during INC of several particles from the ^9Be target nucleus. No preequilibrium
 488 or/and evaporation mechanisms are considered for these reactions by CEM.
 489 There is quite a good agreement of the CEM predictions with the measured
 490 spectra from ^9Be for all products shown in this example: protons (300 MeV p

Figure 15: The same as in Fig. 14, but for the production of ^3He , t , d , and p .

491 + Be), complex particles (t from 300 MeV $p + \text{Be}$ and ^3He and ^4He from 190
 492 and 392 MeV $p + \text{Be}$), and heavier ^6He to ^7Be .

493 Fig. 24 shows examples of similar LF spectra from a carbon nucleus, where
 494 only INC and Fermi breakup reaction mechanisms are considered by our CEM.
 495 CEM produces He and Li from these reaction via Fermi breakup after INC,
 496 while Be and B are probably produced as residual nuclei after emitting several
 497 nucleons during INC from the carbon target nucleus. The general agreement
 498 of the CEM predictions with these measured LF spectra is quite good, taking
 499 into account that no fitting or changing of any parameters in CEM was done;
 500 we used the fixed version of CEM03.03 as implemented in MCNP6.

501 Fig. 25 shows similar examples of LF spectra, namely, double-differential
 502 spectra at 45 degrees of Li, Be, B, and C from ^{14}N and ^{16}O nuclei bombarded
 503 with 70 MeV protons. With these higher mass numbers, we performed calcu-

Figure 16: Examples of measured particle and LF production cross sections from $p + ^{16}\text{O}$ at 600 MeV [47] (symbols) compared with our CEM results for a Fermi breakup cut-off of $A \leq 16$ and $A \leq 12$, as indicated. All the LF from these reactions are calculated by CEM either as final products (residual nuclei) after all possible stages of reaction or via Fermi breakup after INC (Fermi breakup is used for nuclei with $A < 13$ or $A < 17$ instead of using preequilibrium emission and/or evaporation of particles).

lations with CEM03.03 using also $A_{\text{Fermi}} = 14$ and 16, to see how different values affect the final LF spectra. The general agreement of our CEM results with these LF spectra is reasonably good, but not quite as good as seen in Figs. 21 to 24. On the whole, for these particular reactions, CEM03.03 provides a better agreement with the measured LF spectra with $A_{\text{Fermi}} = 12$.

The examples of LF spectra shown in Figs. 21–25 address fragmentation of light targets with proton beams. We present also several examples of LF spectra from nucleus-nucleus reactions. Actually, we have already tested MCNP6

Figure 17: The same as in Fig. 16, but for the production of Li, Be, N, and O isotopes.

512 against almost all available particle and LF data up to ^4He spectra from various
 513 nucleus-nucleus reactions at intermediate energies. As a rule, MCNP6 using its
 514 LAQGSM03.03 event generator describes such spectra quite well (see e.g., Refs.
 515 [11, 13, 14] and references therein). The cases where there is a good agreement
 516 with experimental data are valuable for MCNP6, to verify its predictive power,
 517 but are not so interesting for this study, as they do not address unsolved prob-
 518 lems in the LAQGSM event-generator. One of the worst discrepancies of the
 519 LAQGSM LF spectra with available data found from this V&V of MCNP6 is
 520 shown below in Fig. 26 with dotted lines, namely calculated with the standard
 521 version of LAQGSM invariant spectra of p, d, t, and ^3He from 800 MeV/nucleon
 522 $^{20}\text{Ne} + ^{20}\text{Ne}$ compared with experimental data from Refs. [57, 58]. ^{20}Ne nuclei
 523 are light enough for the subject of our current work, but their mass number

Figure 18: Atomic-number dependence of the fragment-production cross sections from the interactions of ^{20}Ne of 600 MeV/nucleon with H. Experimental data (circles) are by Zeitlin et al. [49]. For comparison, results by the NASA semi-empirical nuclear fragmentation code NUCFRG2 [50] and from a parameterization by Nilsen et al. [51] taken from Tab. III of Ref. [49] are shown as well, as indicated. Our results by CEM03.03 using the “standard” version of the Fermi breakup model ($A_{\text{Fermi}} = 12$) and $A_{\text{Fermi}} = 16$, as well as MCNP6 calculations using CEM03.03 ($A_{\text{Fermi}} = 12$) are plotted with different lines, as indicated.

524 $A > A_{\text{Fermi}} = 12$, therefore LF can be produced by LAQGSM not only with
 525 the Fermi breakup model, when the residual excited nucleus after INC has a
 526 mass number $A < 13$, but also via preequilibrium emission and evaporation, as
 527 well as final residual nuclei after all stages of reactions (see. Fig. 1).

528 Only LF of high and very high energies were measured in those experi-
 529 ments at Bevatron/Bevalac at the Lawrence Berkeley Laboratory [57, 58], and
 530 only products from the fragmentation of the bombarding nuclei were detected.
 531 LAQGSM can reproduce such high-energy portions of spectra only with its coa-
 532 lesence model, as the Fermi breakup model would provide LF of lower energies,
 533 while the preequilibrium emission and evaporation would provide much lower
 534 LF energies; the energies of the LF produced as final “residual nuclei” after all
 535 other stages of reactions would be even much lower. In other words, the ex-

Figure 19: Atomic-number dependence of the fragment-production cross sections from the interactions of 290 MeV/nucleon ^{14}Ne and ^{16}O with C and Al. Experimental data (circles) are by Zeitlin et al. [48]. Our results by LAQGS03.03 using the “standard” version of the Fermi breakup model ($A_{\text{Fermi}} = 12$) are shown with solid lines, and for a cut-off value for A_{Fermi} of 16, with dashed lines, as indicated.

536 perimental data from Refs. [57, 58] are very convenient to test the coalescence
 537 model in LAQGS.

538 As noted in Section 2.2, LAQGS uses fixed values for p_c as determined
 539 by Eq. (1). Results obtained with such “standard” values for p_c are shown in
 540 Fig. 26 with dotted lines: We see that these LAQGS spectra underestimate
 541 the measured data, suggesting that we need to use higher values for p_c , at least
 542 for this particular reaction. As a second test of p_c values, we try to use for this
 543 reaction the values

$$\begin{aligned}
 p_c(d) &= 115 \text{ MeV}/c ; \\
 p_c(t) &= p_c(^3\text{He}) =
 \end{aligned}
 \tag{3}$$

$$= p_c(^4\text{He}) = 175 \text{ MeV}/c ,$$

Figure 20: Atomic-number dependence of the fragment-production cross sections from the interactions of 600 MeV/nucleon ^{20}Ne with C and Al, and 400 MeV/nucleon ^{24}Mg with C and Al. Experimental data (circles) are by Zeitlin et al. [48, 49]. For comparison, at 600 MeV/A, results by the NASA semi-empirical nuclear fragmentation code NUCFRG2 [50] and the microscopic abrasion-ablation model QMSFRG [52], as well as from a parameterization by Nilsen et al. [51] taken from Tabs. III and IV of Ref. [49] are shown with different lines, as indicated. Our results by LAQGS03.03 using the “standard” version of the Fermi breakup model ($A_{\text{Fermi}} = 12$) are shown with solid lines, and for a cut-off value for A_{Fermi} of 16, with dashed lines, as indicated.

544 found to work the best in CEM03.03 in the $300 \text{ MeV} \leq T < 1 \text{ GeV}$ region of
545 incident energies. Results obtained with these values for p_c are shown in Fig.
546 26 with dashed lines: We see that values of p_c defined by Eq. (3) provide too
547 many high energy LF, *i.e.*, these values are too big to provide the best results
548 for LF spectra calculated by LAQGSM for this particular reaction. Finally, we

Figure 21: Examples of measured particle and LF double-differential spectra from $p + {}^9\text{Be}$ at 190 MeV [53], compared with our CEM results (histograms).

try some intermediate p_c values:

$$\begin{aligned}
 p_c(d) &= 120 \text{ MeV}/c ; \\
 p_c(t) &= p_c({}^3\text{He}) = \\
 &= p_c({}^4\text{He}) = 140 \text{ MeV}/c .
 \end{aligned}
 \tag{4}$$

Results calculated with these values are shown with solid lines in Fig. 26: They

Figure 22: Examples of measured particle and LF double-differential spectra from $p + {}^9\text{Be}$ at 300 MeV [53], compared with our CEM results (histograms).

551 agree much better with the measured spectra of d, t, and ${}^3\text{He}$ from this reaction
 552 than the previous two sets of results. Note that the aim of our work is not to fine-
 553 tune the parameters used by the coalescence model in our CEM and LAQGSM
 554 event generators. We may consider such a fine-tuning at a later stage, after
 555 we complete our work on extension of the preequilibrium model to account for
 556 possible emission of LF heavier than ${}^4\text{He}$ at the preequilibrium stage

Figure 23: Examples of measured particle and LF double-differential spectra from $p + {}^9\text{Be}$ at 392 MeV [54], compared with our CEM results (histograms).

of reactions, discussed below. Here, we just show that although the standard versions of our CEM and LAQGSM event generators for MCNP6 provide an overall good agreement of calculated spectra and yields of products from various reactions, a fine-tuning of some of their parameters would allow improving further the agreement of calculated results with available experimental data.

Finally, we mention briefly our preliminary results from recent work [59, 60]

Figure 24: Comparison of CEM03.03 (solid lines) He, Li, Be, and B spectra from 70 MeV p + C with experimental data by Hagiwara et al. [55] (circles) for a natural carbon target. Our calculations were performed for ^{12}C .

to extend the CEM and LAQGSM for accounting possible emission of LF heavier
than ^4He (up to ^{28}Mg) at the preequilibrium stage of nuclear reactions. Fig.
27 shows an example of such results, namely, ^6Li spectra from the reaction 200
MeV p + ^{27}Al measured by Machner et al. [61] (symbols) compared with our
preliminary results by an extended version of CEM, as described in Refs. [59, 60]
(solid lines) and with results by the standard unmodified CEM (dashed lines).

Figure 25: Comparison of Li, Be, B, and C spectra at 45 degrees from 70 MeV p + ^{14}N and ^{16}O measured by Sanami et al. [56] (symbols) with calculations by CEM03.03 using the “standard” version of the Fermi breakup model ($A_{\text{Fermi}} = 12$; solid histograms) and with cut-off values for A_{Fermi} of 16 (dashed histograms) and 14 (long-dashed histograms), as indicated.

569 The aluminum target is relatively light, *i.e.*, such reactions are completely in
 570 the scope of this study. However, in comparison with lighter targets like C, N,
 571 and O discussed above, Al is heavier, the mass number of excited nuclei produced
 572 after INC from such reactions is mostly higher than 12, therefore CEM uses the
 573 preequilibrium and evaporation models to calculate this reaction, in addition to
 574 INC, coalescence, and Fermi breakup models (see Fig. 1).

575 The ^6Li spectra calculated with the standard version of CEM as implemented
 576 at present in MCNP6 shown with dashed histograms came mostly from evapo-
 577 ration of ^6Li from compound nuclei, and also contain a small contribution from
 578 Fermi breakup of excited nuclei with $A \leq A_{\text{Fermi}} = 12$ produced in a few cases
 579 after INC from Al-target, at such a relatively low incident energy of only 200
 580 MeV. As expected, evaporation of ^6Li from compound nuclei together with a
 581 small contribution from Fermi breakup of nuclei with $A \leq A_{\text{Fermi}} = 12$

Figure 26: Comparison of p, d, t, and ^3He spectra at 45, 60, 90, and 130 degrees from 800 MeV/nucleon $^{20}\text{Ne} + \text{NaF}$ measured at the Bevatron/Bevalac at the Lawrence Berkeley Laboratory [57, 58] with calculations by LAQGSM03.03 using its “standard” version of the coalescence model ($p_0 = 0.09 \text{ GeV/c}$ for d, 0.108 GeV/c for t and ^3He , and 0.115 GeV/c for ^4He ; dotted lines) and with modified values of p_0 labeled in legend as “coal1” ($p_0 = 0.15 \text{ GeV/c}$ for d, and 0.175 GeV/c for t, ^3He , and ^4He ; dashed lines), as well as with a second modification of p_0 labeled in legend as “coal2” ($p_0 = 0.12 \text{ GeV/c}$ for d, and 0.14 GeV/c for t and ^3He , and ^4He ; solid lines), as indicated (for simplicity, all calculations were done on a ^{20}Ne target).

582 produced after INC in this reaction do not provide enough high-energy LF
 583 emission, and the calculated ^6Li spectra do not extend to high energies and are
 584 below the measured data. Extension of the preequilibrium model used by CEM
 585 and LAQGSM to account for emission of LF heavier than ^4He as described in
 586 Refs. [59, 60], allows us to produce energetic LF from such reactions, improving
 587 the agreement with many measured LF spectra we tested so far. Of course,
 588 preequilibrium emission of LF is most important for medium and heavy target

Figure 27: Comparison of experimental ${}^6\text{Li}$ spectra at 20, 45, 60, 90, and 110 degrees by Machner et al. [61] (symbols) with calculations by the unmodified CEM03.03 (dashed histograms) and preliminary results with the modified MEM in CEM03.03.F (solid histograms), as indicated.

589 nuclei. But as we see in this example, it also affects significantly such relatively
 590 light nuclei as Al. Our work on extending the preequilibrium model in CEM
 591 and LAQGSM is incomplete. Results from this study will be published in the
 592 future. After completing this work, we may consider a fine-tuning of the A_{Fermi}
 593 parameter of the Fermi breakup model and of the coalescence model parameters
 594 used by the CEM and LAQGSM event generators of MCNP6.

595 4. Conclusion

596 Various fragmentation reactions induced by protons and light nuclei of ener-
 597 gies around 1 GeV/nucleon and below on light target nuclei are studied with the
 598 latest Los Alamos Monte Carlo transport code MCNP6 and with its cascade-
 599 exciton model (CEM) and Los Alamos version of the quark-gluon string model
 600 (LAQGSM) event generators, version 03.03, used as stand-alone codes. On the
 601 whole, MCNP6 and its CEM and LAQGSM event generators describe quite

well all the reactions we tested here, providing good enough agreement with available experimental data. This is especially important for calculations of cross sections of arbitrary products as functions of incident projectile energies, *i.e.*, excitation functions, one of the most difficult tasks for any nuclear reaction model. Our current results show a good prediction by MCNP6 and CEM03.03, used as a stand-alone code, of a large variety of excitation functions for products from proton-induced reactions on N, O, Al, and Si. An older version of CEM, CEM95, was able to predict reasonably well most excitation functions for medium and heavy nuclei-targets, but had big problems in calculating some excitation functions for light nuclei [62].

CEM and LAQGSM assume that intermediate-energy fragmentation reactions on light nuclei occur generally in two stages. The first stage is the intranuclear cascade (INC), followed by the second, Fermi breakup disintegration of light excited residual nuclei produced after INC. Both CEM and LAQGSM also account for coalescence of light fragments (complex particles) up to ^4He from energetic nucleons emitted during INC.

We investigate the validity and performance of MCNP6, CEM, and LAQGSM in simulating fragmentation reactions at intermediate energies. We find that while the fixed “default” versions of CEM03.03 and LAQGSM03.03 in MCNP6 provide reasonably good predictions for all reactions tested here, a fine-tuning of the A_{Fermi} parameter in the Fermi breakup model and of momentum cut-off parameters in the coalescence model may provide a better description of some experimental data. We may consider such a fine-tuning of these and other CEM and LAQGSM parameters later, after we complete our work [59, 60] on extending the preequilibrium model in CEM and LAQGSM to account for possible emission of light fragments heavier than ^4He (up to ^{28}Mg) at this stage of reactions.

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