Preequilibrium Emission of Light Fragments in Spallation Reactions

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The ability to describe production of light fragments (LF) is important for many applications, such as cosmic-ray-induced single event upsets (SEUs), radiation protection, and cancer therapy with proton and heavy-ion beams. The cascade-exciton model (CEM) and the Los Alamos version of the quark-gluon string model (LAQGSM) event generators in the LANL transport code MCNP6, describe quite well the spectra of fragments with sizes up to 4He across a broad range of target masses and incident energies (up to ∼ 5 GeV for CEM and up to ∼ 1 TeV/A for LAQGSM). However, they do not predict the high-energy tails of LF spectra heavier than 4He well. Most LF with energies above several tens of MeV are emitted during the precompound stage of a reaction. The current versions of our event generators do not account for precompound emission of LF larger than 4He. The aim of our work is to generalize the precompound model to include such processes, leading to increased predictive power of LF production. Extending the model in this way provides preliminary results that have much better agreement with experimental data.

I. INTRODUCTION

Emission of light fragments (LF) from nuclear reactions is an interesting open question. Different reaction mechanisms contribute to their production; the relative roles of each, and how they change with incident energy, mass number of the target, and the type and emission energy of the fragments is not completely understood.

None of the available models are able to accurately predict emission of LF from arbitrary reactions. However, the ability to describe production of LF (especially at energies > 30 MeV) from many reactions is important for different applications, such as cosmic-ray-induced single event upsets (SEUs), radiation protection, and cancer therapy with proton and heavy-ion beams. The cascade-exciton model (CEM) [1, 2] version 03.03 and the Los Alamos version of the quark-gluon string model (LAQGSM) [2, 3] version 03.03 event generators in the Monte-Carlo n-particle transport code version 6 (MCNP6) [4], describe quite well the spectra of fragments with sizes up to 4He across a broad range of target masses and incident energies (up to ∼ 5 GeV for CEM and up to ∼ 1 TeV/A for LAQGSM). However, they do not predict the high-energy tails of LF spectra heavier than 4He. Most LF with energies above several tens of MeV are emitted during the precompound stage of a reaction. The current versions of the CEM and LAQGSM event generators do not account for precompound emission of these heavier LF.

The aim of our work is to extend the precompound model in the codes to include such processes, leading to an increase of predictive power of LF-production in MCNP6. This entails upgrading the modified exciton model currently used at the preequilibrium stage in CEM and LAQGSM. It will also include expansion and examination of the coalescence and Fermi break-up models used in the precompound stages of spallation reactions within CEM and LAQGSM. Extending our models to include emission of fragments heavier than 4He at the precompound stage already gives preliminary results with much better agreement with experimental data.

II. THEORETICAL BACKGROUND

Our models consider that a reaction begins with the IntraNuclear Cascade, referred to as the INC. The incident particle or nucleus (in the case of LAQGSM) enters the target nucleus and begins interacting with nucleons, scattering off them and also often creating new particles in the process. The incident particle and all newly created particles are followed until they either escape from the nucleus, are absorbed, or, for nucleons, reach a threshold energy (roughly 10-30 MeV) and are then considered “absorbed” by the nucleus.

The preequilibrium stage uses the modified exciton model (MEM) to determine emission of protons, neutrons, and fragments up to 4He from the residual nu-
We discuss the MEM in more detail below. This stage can have a highly excited residual nucleus undergoing dozens of exciton transitions and particle emissions. The preequilibrium stage ends when the residual nucleus is just as likely to have a \( \Delta n = +2 \) exciton transition as a \( \Delta n = -2 \) exciton transition.

In the evaporation stage, neutrons and protons in the residual nucleus can “evaporate,” either singly or as fragments. The CEM evaporation stage is modeled with a modification of the Furihata’s generalized evaporation model code (GEM2) \(^6\), and includes light fragments up to \(^{28}\)Mg.

During and after evaporation, the code looks to see if we have an isotope that has \( Z \geq 65 \) and is fissionable. If it is, and there is fission, then the code also allows evaporation from the fission fragments.

There are two models that are not directly parts of this progression: coalescence and Fermi break-up. The INC stage only emits neutrons, protons, and pions (and other particles, when using LAQGSM at high energies), so the coalescence model “coalesces” some of the INC neutrons and protons into larger fragments, by comparing their momenta. If their momenta are similar enough then they coalesce. The current coalescence model can only coalesce up to \(^4\)He fragments, the same as the preequilibrium stage. The Fermi break-up is an oversimplified multifragmentation model that is fast and accurate for small atomic numbers; in the current CEM model it is used when any residual nucleus or fragment has a mass number less than 13.

The MEM used by CEM and LAQGSM \(^6\) \(^5\) calculates \( \Gamma_j \), the emission width (or probability of emitting particle fragment \( j \)) as

\[
\Gamma_j(p, h, E) = \int_{V_j}^{E-B_j} \lambda_j^p(p, h, E, T) dT,
\]

where the partial transmission probabilities, \( \lambda_j^p \), are equal to

\[
\lambda_j^p(p, h, E, T) = \frac{2s_j + 1}{\pi^2 h^2 \mu_j^p R(p, h)} \times \\
\omega(p-1, h, E-B_j-T) T \sigma_{inv}(T).
\]

Eq. (2) describes the emission of neutrons and protons. For complex particles, the nuclear level density \( \omega \) becomes more complicated and an extra phase-space factor \( \gamma_j \) must be introduced:

\[
\gamma_j \approx p_j^3 (p_j/A)^{p_j-1}.
\]

Eq. (3) for \( \gamma_j \) is a only a rough estimation that we improve by parameterizing it over a mesh of residual nuclei energy and mass numbers in our codes \(^10\). As the MEM uses a Monte-Carlo technique to solve the master equations describing the behavior of the nucleus at the preequilibrium stage (see details in \(^7\)), it is very easy to extend the number of types of possible LF that can be emitted during this stage. We generalize the MEM to consider the possibility of emission up to 66 types of nucleons and LF, up to \(^{28}\)Mg. As a starting point, for the inverse cross sections, Coulomb barriers, and binding energies of all LF we use the approximations adopted by GEM2 \(^6\).

### III. RESULTS

Extending the Fermi break-up model to include heavier LF (up to \( A = 16 \)) allows us to use it for nuclei with \( A > 12 \), yielding increased accuracy for reactions with light targets. Below are examples of calculations by CEM (with the expanded Fermi break-up model) compared to experimental data \(^8\) \(^9\).

![FIG. 1](image1.png)

![FIG. 2](image2.png)
achieve good agreement with experimental results for these light targets.

Expanding the MEM to include heavier LF (up to ²⁸Mg) yields increased accuracy for several reactions we investigate. Figure 3 compares new simulations from our expanded model with data by Machner et al. [5] for 200 MeV p + ²⁷Al.

We also find that the integral spectra for n, p, d, t, ³He, and ⁴He (not shown), are not significantly impacted by this LF emission expansion.

Figure 4 compares our results for 1200 MeV p + natNi with new data by Budzanowski et al. [8].

Similar results for different LF spectra are obtained for several other reactions (see, e.g., [11]).

Our results indicate that expanding the MEM to include LF preequilibrium emission significantly increases accuracy of the high-energy spectra compared to experimental data.

IV. CONCLUSIONS

Extending the CEM model to include emission of light fragments (LF) heavier than ⁴He (up to ²⁸Mg) in the preequilibrium stage results in significantly improved accuracy compared to experimental data for several reactions, especially in the high-energy tails of the spectra.

Future work includes finding a global parametrization for γβ, incorporating the expanded event generators into MCNP6, adding coalescence of heavier fragments, further exploring Fermi break-up, and upgrading the evaporation model.

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