Production of Heavy Clusters with an Expanded Coalescence Model in CEM

Leslie M. Kerby,1,2 Stepan G. Mashnik1

1Los Alamos National Laboratory, Los Alamos, New Mexico USA
2University of Idaho, Idaho Falls, Idaho USA
leslie31415@gmail.com

INTRODUCTION

The production of heavy clusters in nuclear reactions is important in a wide variety of applications: radiation shielding, space engineering and design, medical physics, accelerator design, and more. According to the Cascade Exciton Model (CEM) [1, 2], there are three ways high-energy heavy clusters can be produced. The first way is via coalescence of nucleons produced in the IntraNuclear Cascade (INC). The second way is via the preequilibrium model. The last way is via Fermi breakup. Previous work in CEM examines the impact of expansions of the preequilibrium model and Fermi breakup model on heavy cluster production [3–7]. The present work studies the impact of expanding the coalescence model on heavy cluster spectra. CEM03.03 [2], the default event generator in the Monte Carlo N-Particle transport code version 6 (MCNP6) [3] for intermediate-energy nuclear reactions, is capable of producing light fragments up to 4He in its coalescence model. In the present study, we have expanded the coalescence model to be able to produce up to 7Be. Preliminary results are promising.

BACKGROUND

When the cascade stage of a reaction is completed, CEM uses the coalescence model described in Ref. [9, 10] to “create” high-energy d, t, 3He, and 4He by final-state interactions among emitted cascade nucleons outside of the target nucleus. The coalescence model used in CEM is similar to other coalescence models for heavy-ion-induced reactions. The main difference is that instead of complex-particle spectra being estimated simply by convolving the measured or calculated inclusive spectra of nucleons with corresponding fitted coefficients, CEM03.03 uses in its simulations of particle coalescence real information about all emitted cascade nucleons and does not use integrated spectra. (Note that the coalescence introduced recently in the Liège intranuclear cascade (INCL) [11-14], is in a way similar to the coalescence considered by CEM as proposed in Ref. [9, 10], with the main contrast being that INCL considers coalescence of INC nucleons on the border of a nucleus, inside the target-nucleus, while CEM coalesces INC nucleons outside the nucleus.) We assume that all the cascade nucleons having differences in their momenta smaller than \( p_c \) and the correct isotopic content form an appropriate composite particle. The coalescence radii \( p_c \) as used in CEM03.03 are:

\[
\begin{align*}
    p_c(d) &= 90 \text{ MeV}/c ; \\
    p_c(t) &= p_c(3\text{He}) = 108 \text{ MeV}/c ; \\
    p_c(4\text{He}) &= 115 \text{ MeV}/c .
\end{align*}
\]

If several cascade nucleons are chosen to coalesce into composite particles, they are removed from the distributions of nucleons and do not contribute further to such nucleon characteristics as spectra, multiplicities, etc.

COALESCENCE EXPANSION

The Coalescence Model in CEM03.03 allows for coalescence up to 4He. We have expanded this to additionally allow for the coalescence of 6He, 6Li, 7Li, and 7Be.

CEM03.03 uses the simplest version of the coalescence model [9, 10] and checks only the momenta of nucleons emitted during the cascade stage of reactions, without checking their coordinates.

The momentum, \( p \), of each nucleon is calculated relativistically from its kinetic energy, \( E \) (CEM03.03 provides in its output files the energy of particles, but not their momenta). Coalescence occurs if each nucleon in the group has \( |\Delta p| \leq p_c \), where \( \Delta p \) is defined as the difference between the nucleon momentum and the average momentum of all nucleons in the group.

The coalescence model of CEM03.03 first checks all nucleons to form 2-nucleon pairs, their momenta permitting. It then checks if an alpha particle can be formed from two 2-nucleon pairs (either from 2 n-p pairs or from a n-n and p-p pair). After this it checks to see if any of the 2-nucleon pairs left can combine with another nucleon to form either tritium or 3He. And lastly, it checks to see if any of these 3-nucleon groups (tritium or 3He) can coalesce with another nucleon to form 4He.

The expanded coalescence model then takes these 2-nucleon pairs, 3-nucleon (tritium or 3He only) groups, and 4He to see if they can coalesce to form heavy clusters. 4He can coalesce with a 3-nucleon group to form either 7Be or 7Li. Two 3-nucleon groups can coalesce to form either 6Li or 6He. And 4He can coalesce with a 2-nucleon pair to form either 6Li or 6He. All coalesced nucleons are removed from the distributions of nucleons so that our coalescence model conserves both atomic- and mass-numbers. In addition, this expansion requires an insignificant amount (2–3 %) of increased computation time.

For additional details of the Coalescence Model expansion, see Ref. [13].
Coalescence Parameter $p_c$

As mentioned above, $p_c$ determines how dissimilar the momenta of nucleons can be and still coalesce. $p_c$ was expanded to also include a value for heavy clusters, or light fragments (LF): $p_c(LF)$. Our new $p_c$’s for incident energies, $T$, less than 300 MeV or greater than 1000 MeV are:

\begin{align*}
    p_c(d) &= 90 \text{ MeV/c} ; \\
    p_c(t) &= p_c(3^4\text{He}) = 108 \text{ MeV/c} ; \\
    p_c(3^4\text{He}) &= 130 \text{ MeV/c} ; \\
    p_c(LF) &= 175 \text{ MeV/c} .
\end{align*}

And for 300 MeV < $T$ < 1000 MeV

\begin{align*}
    p_c(d) &= 150 \text{ MeV/c} ; \\
    p_c(t) &= p_c(3^4\text{He}) = 175 \text{ MeV/c} ; \\
    p_c(3^4\text{He}) &= 205 \text{ MeV/c} ; \\
    p_c(LF) &= 250 \text{ MeV/c} .
\end{align*}

Note that the $p_c(3^4\text{He})$ was also increased compared to the old $p_c$ values. Too many alpha particles were lost (coalesced into heavy clusters), and therefore we compensated by increasing the coalescence of $3^4\text{He}$.

RESULTS AND ANALYSIS

Examples of results of our coalescence expansion are displayed in Figs. 1–3. The upgraded CEM03.03F without coalescence expansion (blue solid lines) and the upgraded CEM03.03F with coalescence expansion (red dashed lines) are compared with experimental data (green circles). This coalescence expansion analysis is part of a larger project [3–7] aimed at producing high-energy light fragments in spallation reactions. CEM03.03F refers to the upgraded CEM03.03 code, aimed at producing high-energy light fragments in spallation reactions. CEM03.03F refers to the upgraded CEM03.03 code, and the red dashed lines contain both of these improvements plus the coalescence expansion. The blue solid lines contain both of these improvements over the original CEM03.03, and the red dashed lines contain both of these improvements plus the coalescence expansion.

Fig. 1 displays fragment production spectra of $3^6\text{He}$ and $3^6\text{Li}$ for the reaction 1200 MeV p + $^{197}\text{Au}$. Experimental data by Budzanowski et al. [16] (green circles) are compared with results from CEM03.03F without coalescence expansion (blue solid lines) and CEM03.03F with coalescence expansion (red dashed lines). The coalescence expansion increases the production of high-energy $3^6\text{He}$ and $3^6\text{Li}$, and improves agreement with experimental data.

Fig. 2 displays the fragment production spectra of $3^7\text{Li}$ and $3^7\text{Be}$ for the reaction 480 MeV p + $^{197}\text{Ag}$. Experimental data by Green et al. [17] (green circles) are compared with results from CEM03.03F without coalescence expansion (blue solid lines) and CEM03.03F with coalescence expansion (red dashed lines). Again, the coalescence expansion increases the production of heavy clusters, and improves agreement with experimental data.

These reactions also highlight how the coalescence can produce heavy clusters not just of high-energy, but also of low- and moderate-energy, thus improving agreement with experimental data in these energy regions as well.

Fig. 3 displays experimental results of the reaction 480 MeV p + $^{197}\text{Ag} \rightarrow 3^6\text{Li}$ by Green et al. [17] (green circles), compared with simulations from results from CEM03.03F without coalescence expansion (blue solid lines), CEM03.03F with coalescence expansion (red dashed lines), and the original CEM03.03 (brown dashed-dotted lines). Even without the coalescence expansion, CEM03.03F (which contains a preequilibrium expansion and a total reaction cross section improvement) yields much better results than CEM03.03 without any of these improvements. Adding the coalescence expansion produces even better results.

Similar results for many other reactions induced by protons, neutrons, and heavy ions (the last are simulated with LAQGSM03.03 [2], but with an extended coalescence model as described in Ref. [18]) and further discussions can be found in Refs. [15, 18].
Fig. 2. Comparison of experimental data by Green et al. [17] (green circles) for the production of $^7$Li and $^7$Be at an angle of 40° from the reaction 480 MeV $p + ^{101}$Ag, with results from CEM03.03F without coalescence expansion (blue solid lines) and CEM03.03F with coalescence expansion (red dashed lines).

CONCLUSIONS

Expanding the coalescence model within CEM yields increased production of heavy clusters in nuclear spallation reactions, particularly in the high-energy region, but also in the low- and moderate-energy regions. Preliminary results indicate this coalescence expansion yields improved agreement with experimental data. We plan to implement these upgrades into MCNP6.

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