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NUCFRG3: Light ion improvements to the nuclear fragmentation model

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ABSTRACT

Light ion improvements to the nuclear fragmentation model, NUCFRG, are reported. Improvements include the replacement of the simple light ion production model with a light ion coalescence model and an improved electromagnetic dissociation (EMD) formalism. Prior versions of the model provide reasonable overall agreement with measured data; however, those versions lack a physics-based description for coalescence and EMD. The version reported herein, NUCFRG3, has improved the theoretical descriptions of these mechanisms and offers additional benefits, such as the capability to calculate EMD cross-sections for single deuteron, triton, helion, and alpha particle emission. NUCFRG3 model evaluation and validation show that the predictive capability has been improved and strengthened by the light ion physics-based changes. Based on increased capability and better theoretical grounding, it is recommended that NUCFRG3 replace its predecessors for space radiation assessments and other applications.

1. Introduction

Development of the NUCFRG (NUClear FRaGmentation) series of the nuclear fragmentation model began at NASA Langley Research Center in the mid-1980s in order to provide a fast, accurate, and reliable algorithm for generating nuclear fragmentation cross-section databases for galactic cosmic ray (GCR) transport and shielding studies relevant to future NASA missions. These models use a semiempirical nuclear collision formalism based upon an abrasion–ablation model of heavy-ion fragmentation and provide a reasonable representation for many of the measured elemental and isotopic production cross-sections found in the literature. Described herein is the third revision of the NUCFRG model, namely NUCFRG3.

The first version of the model [1,2] was based upon the classical geometric abrasion–ablation model of Bowman et al. [3] as extended by Gosset et al. [4]. Major improvements in the abrasion model used in NUCFRG over the Bowman and Gosset abrasion models included the use of an average transmission factor for the projectile and target nuclei at a given impact parameter to account for the finite mean free path in nuclear matter. Also, for use in the ablation stage of the reaction, a second-order correction was implemented in the surface energy term used to estimate the prefragment excitation energies. The first revision to NUCFRG, named HZEFRG1 (High charge (Z) and Energy FRaGmentation), introduced electromagnetic dissociation (EMD) into the model and incorporated an energy dependent mean free path [5].

The most recent version in the series, NUCFRG2, was published in 1994 [6,7]. Major improvements included evaluating the transmission factor in the overlap region at the maximum overlap in the interaction zone. Coulomb trajectories for the collision were incorporated, replacing the straight line trajectories used previously. The spectator nucleons in the interaction zone are now assumed to be poorly bound to the spectators of the abraded fragment outside the interaction zone and undergo pre-equilibrium emission. A unitarity correction was made for targets more massive than copper. Finally, a correction to the semiempirical surface distortion energy was made for light projectiles.

The continued development of an accurate high-energy heavy-ion cross-section model is necessary to obtain reliable space radiation shielding and health risk assessments when using space radiation transport codes. NUCFRG2 predicts nuclear fragmentation cross-sections from the collisions of heavy nuclear projectiles ($A \geq 4$) and provides the nuclear fragmentation cross-sections for some versions of the particle transport code HZETRN (High charge (Z) and Energy TRaNsport) [8–10], which is a computational tool used in space radiation studies and shield design. In addition,

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NUCFRG2 cross-sections are used in the event generator of the Monte Carlo radiation transport code HETC-HEDS (High Energy Transport Code-Human Exploration and Development of Space) [11]. HETC-HEDS facilitates three-dimensional analyses of space radiation shielding scenarios. Furthermore, the abrasion–ablation model, on which NUCFRG2 is based, has been incorporated into Geant4 (GEometry ANd Tracking) [12], which is a software toolkit designed for detector and physics simulations and is used for various applications, which include high energy physics, astrophysics, medical physics, and radiation protection [13].

Space-related assessments and applications are partially dependent on light ion ($A \leq 4$) nuclear reactions and light ion production in the GCR spectrum. The National Council on Radiation Protection and Measurements (NCRP) Report no. 153 [14] states there is a need to "improve existing nuclear interaction databases for properly assessing risk and concomitant shielding requirements, especially for neutrons and light ions" and later to "develop models to accurately predict neutron and light ion (hydrogen and helium isotopes) spectra from nucleon-nucleus and nucleus-nucleus collisions of GCR ions on relevant target atoms" [14]. Light ion production mechanisms include, but are not limited to nuclear abrasion, ablation, coalescence, and electromagnetic dissociation (EMD). In this work, the light ion physics capabilities of NUCFRG2 have been extended and improved with the incorporation of new physics-based coalescence and EMD models. This improved version will be referred to as NUCFRG3. The updated models have been validated against available experimental data. However, the number of experimental results, including those that are not applicable to space applications, is small compared to the number of target, energy, projectile, and fragment combinations found in GCR interactions.

In NUCFRG3, there are two main improvements that have been made to the light ion production models. First, light ion formation through the coalescence of nucleons has been added to the abrasion–ablation model. Second, the EMD model has been extended to predict not only nucleon emission, but deuteron, triton, helion, and alpha emission as well. These improvements will be discussed in the subsequent sections and will be accompanied by their detailed formalisms. It is important to note that while the coalescence and EMD models presented herein have been incorporated into NUCFRG3, both of the models may also be incorporated into other nuclear fragmentation codes.

Changes will then be evaluated in order to determine if the resulting NUCFRG3 model is more accurate in terms of cross-section predictions for use in space radiation transport calculations. Two primary issues are of interest in this assessment: quantifying the uncertainty of the NUCFRG2 and NUCFRG3 models against the available data relevant to space radiation analysis and assessing the validity of the models in regions of phase space away from the available data. The first issue will be addressed by use of quantitative validation metrics in the comparisons of the model results to data. For the second, the completeness of the available data will be assessed, and the theoretical foundations of the two models will be compared.

2. Coalescence model

In NUCFRG2, light ions ($A \leq 4$) can be produced during the abrasion stage of the model only by being the heaviest fragment produced. The leftover nucleons from the abrasion are then used to make as many alpha particles as numerically possible. Any nucleons remaining after forming alphas are considered free nucleons. Light ions can also be created in the ablation stage as the final state particle after all excitation energy was dissipated through nucleon removal. This simple model largely ignores the possibility of non-alpha light ion production. A production mechanism for light ions is through coalescence, in which nucleons that are close together in phase space will be coalesced into light ions by the strong nuclear force.

Properly implementing the coalescence formalism into NUCFRG3 required some internal modifications to the NUCFRG2 code in order to remove the existing simplified light ion production scheme previously employed and incorporated. The coalescence formalism that has been developed is the first version. As such, it incorporates some assumed parameters that need further study and theoretical formulation and justification, such as the multiplicities of the light ions produced.

The coalescence model developed for NUCFRG3 is a modified version of the model published by Awes et al. [15], where the composite particle multiplicity distribution is

$$\frac{d^3\mathcal{N}(Z,N)}{dp^3} = \frac{\overline{m}_{\mathrm{A}}}{N!Z!}\left(\frac{4\pi}{3}P_0^3\gamma\right)^{A-1}\left(\frac{N_\mathrm{P}+N_\mathrm{T}}{Z_\mathrm{P}+Z_\mathrm{T}}\right)^N\left[\frac{d^3\mathcal{N}(1,0)}{dp^3}\right]^A. \tag{1}$$

Here, Z, N, and A are the composite (coalesced light ion) particle atomic number, neutron number, and mass number, respectively, $\overline{m}_{\mathrm{A}}$ is the mean multiplicity of the composite particle (A), γ is the usual relativistic gamma factor, P_0 is the coalescence radius in momentum space, $N_{\mathrm{P,T}}$ is the projectile nucleus (P) and target nucleus (T) neutron number, $Z_{\mathrm{P,T}}$ is the projectile nucleus (P) and target nucleus (T) atomic number, p is the momentum per nucleon, and $d^3\mathcal{N}(1,0)/dp^3$ is the differential nucleon multiplicity distribution. The coalescence radius, P_0, is the radius in momentum space such that nucleons with relative momentum less than P_0, located spatially close together and traveling in the same direction, are assumed to coalesce to form light ions with mass numbers $2 \leq A \leq 4$.

In NUCFRG2, all fragmentation yields are calculated for the projectile alone. Target quantities are calculated by interchanging the target and projectile in the code. Hence, a modified form of Eq. (1) is re-derived as

$$\frac{d^3\mathcal{N}(Z,N)}{dp_{\mathrm{A}}^3} = \frac{\overline{m}_{\mathrm{A}}}{N!Z!}\left(\frac{4\pi}{3}P_0^3\gamma\right)^{A-1}\left(\frac{N_\mathrm{P}}{Z_\mathrm{P}}\right)^N\left[\frac{d^3\mathcal{N}(1,0)}{dp^3}\right]^A \tag{2}$$

where subscript A refers to the composite particle. The multiplicity term in Eq. (2) can be expressed in terms of the reaction cross-section, σ_R, as

$$\frac{d^3\mathcal{N}}{dp^3} = \frac{1}{\sigma_R}\frac{d^3\sigma}{dp^3} \tag{3}$$

where σ is defined as the yield cross-section for a fragment type. Combining Eqs. (2) and (3) yields

$$\frac{d^3\mathcal{N}(Z,N)}{dp_{\mathrm{A}}^3} = \frac{1}{\sigma_R}\frac{d^3\sigma(Z,N)}{dp_{\mathrm{A}}^3} = \frac{\overline{m}_{\mathrm{A}}}{N!Z!}\left(\frac{4\pi}{3}P_0^3\gamma\right)^{A-1}\left(\frac{N_\mathrm{P}}{Z_\mathrm{P}}\right)^N\left[\frac{1}{\sigma_R}\frac{d^3\sigma(1,0)}{dp^3}\right]^A. \tag{4}$$

Therefore

$$\frac{d^3\sigma(Z,N)}{dp_{\mathrm{A}}^3} = \frac{\overline{m}_{\mathrm{A}}}{N!Z!}\left(\frac{4\pi}{3\sigma_R}P_0^3\gamma\right)^{A-1}\left(\frac{N_\mathrm{P}}{Z_\mathrm{P}}\right)^N\left[\frac{d^3\sigma(1,0)}{dp^3}\right]^A. \tag{5}$$

For NUCFRG3, the coalescence radius must be expressed in terms of total yields (cross-sections) rather than differential ones. To obtain the required form from Eq. (5), integrate over the momentum distributions, where

$$dp_{\mathrm{A}}^3 = A^3 d^3p. \tag{6}$$

Experimentally, Greiner et al. [16] found that projectile fragments, in the projectile rest frame, have a Gaussian momentum