# DEVELOPMENT OF A MONTE CARLO RADIATION TRANSPORT CODE SYSTEM FOR HEDS: STATUS UPDATE

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**Abstract**

Modifications of the Monte Carlo radiation transport code HETC are underway to extend the code to include transport of energetic heavy ions, such as are found in the galactic cosmic ray spectrum in space. The new HETC code will be available for use in radiation shielding applications associated with missions, such as the proposed manned mission to Mars. In this work the current status of code modification is described. Methods used to develop the required nuclear reaction models, including total, elastic and nuclear breakup processes, and their associated databases are also presented. Finally, plans for future work on the extended HETC code system and for its validation are described.

## I. Background

Galactic cosmic rays (GCR) and occasional, but intense, fluxes of solar energetic particles (SEP) present severe radiation hazards to manned planetary exploration, such as the proposed human mission to Mars. Although the major uncertainty in estimating crew risk to these radiations is related to the biological response to HZE (high charge and energy) ions in the GCR environment, a significant uncertainty (possibly a factor of two) may be contributed by current radiation transport models and methods used in predicting secondary particle fluxes and their spectra behind shielding[1]. The current uncertainty estimates are so large that simply adding more shielding to account for them imposes severe weight penalties and is not a viable option. Therefore research directed toward reducing the uncertainties is required.

In this work we are developing a radiation transport code system for deep space applications based on Monte Carlo methods. This is the methodology most commonly used in a variety of technical areas for high-energy radiation transport, but has not been previously applied in addressing these space radiation issues. This transport method has inherent capabilities - namely, 3-D transport, modular programming, and detailed output - that are very important for human exploration applications. The code used herein is the High Energy Transport Code (HETC).[2]

Most of the work involves extending HETC to include heavy-ion transport, which is needed for human exploration and development of space (HEDS) applications to transport the heavy-ion component of the GCR environment. This is being accomplished by incorporating heavy-ion nuclear collisions models into HETC. Also, we plan to update the nucleon/pion nuclear collision model in HETC to incorporate the most accurate models currently in use worldwide. This new heavy-ion/nucleon-meson transport code, HETC/HEDS, will be coupled with other transport codes specialized for low-energy neutron transport (MORSE) and electron-photon transport (EGS) to provide a full-capability Monte Carlo radiation transport "code

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system" for HEDS applications. The following sections describe the work carried out to date in performing these modifications.

**II. Needed Modifications to HETC**

While HETC has had wide application, it is not suitable for all HEDS applications in its present form because it does not incorporate the transport of heavy ions, which are an important component of the GCR environment for HEDS radiation protection assessments. Therefore, a major part of the work being carried out focuses on extending HETC to include heavy ion nuclear interaction models and the associated software modifications needed for heavy ion tracking.

Unfortunately, a single, complete heavy-ion nuclear-collision model, capable of rapidly and accurately predicting double differential energy-angle secondary spectra for all of the ions, energies, and target materials of interest, does not exist. Therefore, we resort to using several models that address different aspects of nucleus-nucleus collisions. As GCR ions are transported, the distance to the next nuclear interaction must be determined. This requires knowing total cross sections (sum of elastic and reaction cross sections) for nucleus-nucleus collisions over energies ranging from several MeV/nucleon up to several GeV/nucleon in order to estimate the mean free path (usually several cm) for nuclear collision. The methodology used to calculate these cross sections is described in the next section. Since these heavy ions are highly charged (ionized), they also lose energy through a myriad of collisions with orbital electrons of the atoms in the target medium. This energy loss must also be accounted for in the transport code. Once the collision occurs, it must be determined if it is an elastic or nonelastic collision. Nonelastic collisions at typical GCR energies are usually fragmentation or spallation events, where one or both nuclei breakup as a result of the collision. Since no single model exists that specifies the directions and energies of all secondary particles produced in collisions of all incident and target nuclei at all energies of interest, a hybrid one is being developed, as discussed in the next section.

Software interfaces for the extended version of HETC containing heavy-ion transport and updated nucleon and pion collision models (designated here as HETC/HEDS) must be provided so that it can be coupled with low-energy neutron transport and electron-photon transport codes. This provides a complete Monte Carlo transport code system for HEDS, capable of transporting all particle types (protons, heavy ions, neutrons, pions, muons, electrons, positrons, and photons) over all energy ranges of interest for GCR (and SEP) induced environments.

The nuclear models to be incorporated into HETC/HEDS are not applicable for low-energy (<20 MeV) neutron interactions, but several well-tested and widely used transport codes are available that provide neutron transport from 20 MeV down to thermal energies and take into account the production and transport of secondary gamma-rays from inelastic scattering and capture reactions. We plan to deliver the code system with MORSE[3] as the low-energy neutron transport code although the interface with HETC/HEDS will be such that other codes, such as the Los Alamos MCNP code, could also be used.

The HETC/HEDS code system will also allow coupling with the EGS (Electron-Gamma Shower) Monte Carlo code[4] for (optionally) calculating the electromagnetic cascade induced by neutral-pion decay. The HETC/HEDS, MORSE, and EGS transport codes will be interfaced with a common 3-D combinatorial geometry (CG). The CG methodology allows complex configurations to be modeled based on logical combinations of simple volumes (spheres, boxes, cones. etc.). This type of geometry module has been well tested and is often used with these transport codes.

We will also provide the HETC/HEDS-MORSE-EGS code system for HEDS applications with a general source module for ambient GCR and SEP proton and heavy-ion environments. This module will allow users to specify GCR and SEP sources to be used as input. There are two reasons for incorporating this specialized source module: as a convenience to users, and because special techniques are needed to ensure that the Monte Carlo energy selections from spectra over the large GCR energy range (~10 MeV/nucleon - 100 GeV/nucleon) are made accurately.

## III. Status of Modifications

Modifications to the HETC code are in progress. Those completed or nearly completed include: 1) The range energy tables for all nuclides have been incorporated and debugging processes have begun; 2) The interfaces with the cross sections and collision models have been defined and programmed into the heavy ion transport system; 3) The geometry module has been interfaced with the heavy ion transport module. Note that the interfaces mentioned in 2) still require the appropriate collision models/data as inputs. These data needs are currently being addressed as described below.

### *Nuclear Database Development*

Nuclear databases needed include total cross sections, which enable collision mean free paths to be determined, and double-differential secondary particle production cross sections (energy and angle for every secondary particle). A suitable model for the total cross section has been developed for use in the HETC/HEDS code system. It is described below. Double-differential cross sections for secondary particle production do not exist for most projectile-target-beam energy combinations of interest, either as experimental data or as theoretical formulations. Hence, models must be adapted from other applications or developed specifically for use in this code system. The present status of fragmentation database development is also described below.

**1. Total Cross Sections.** Since there are essentially no measured data in existence for total cross sections from nucleus-nucleus collisions, they must be modeled using nuclear theory. During the 1970's and early 1980's, quantum mechanical optical potential models, based on multiple scattering theory, were developed at NASA Langley Research Center[5-7] for use in generating databases of nucleon-nucleus and nucleus-nucleus total and reaction cross sections for GCR heavy ion transport. The predicted cross sections were found to be in excellent agreement with measurements of total and reaction cross sections for nucleon-nucleus collisions and for nucleus-nucleus reaction cross sections for energies above ~50 Mev/nucleon. At lower energies there were tendencies for both the predicted total and reaction cross sections to be smaller than the measured values, especially for incident nucleons and light ions such as deuterons. As the projectile kinetic energies decreased, the differences between predicted and measured values increased. Nevertheless, tabulated values of these cross sections for energies between 25 MeV/nucleon and 22.5 GeV/nucleon were published.[6,8,9]

In subsequent work at NASA Langley, Tripathi developed a semiempirical formulation of nuclear reaction cross sections which was accurate down to energies as low as ~ 1 MeV/nucleon.[10,11] Hence, it was decided to improve the low energy predictions for the total cross sections to be used in HETC by scaling the reaction cross sections of Tripathi using ratios of the total-to-reaction cross sections obtained from the earlier quantum mechanical optical model[7] developed at NASA Langley. Thus, the total cross section is estimated from

$$\sigma_{TOT} = R\,\sigma_R(\text{Tripathi}) \tag{1}$$

where R is the optical model cross section ratio given by

$$R = \sigma_{TOT}(\text{optical})/\sigma_R(\text{optical}) \tag{2}$$

Sample results are displayed in Figures 1 and 2 for carbon-carbon scattering and for iron-lead scattering.

These nuclear systems were chosen for illustrative purposes since they represent systems involving lighter and heavier pairs of nuclei of interest in GCR transport. Displayed are the results from Townsend et al[8] (labeled "Optical") and the predictions obtained using Eq. (1) (labeled "This Work"). Note that the cross

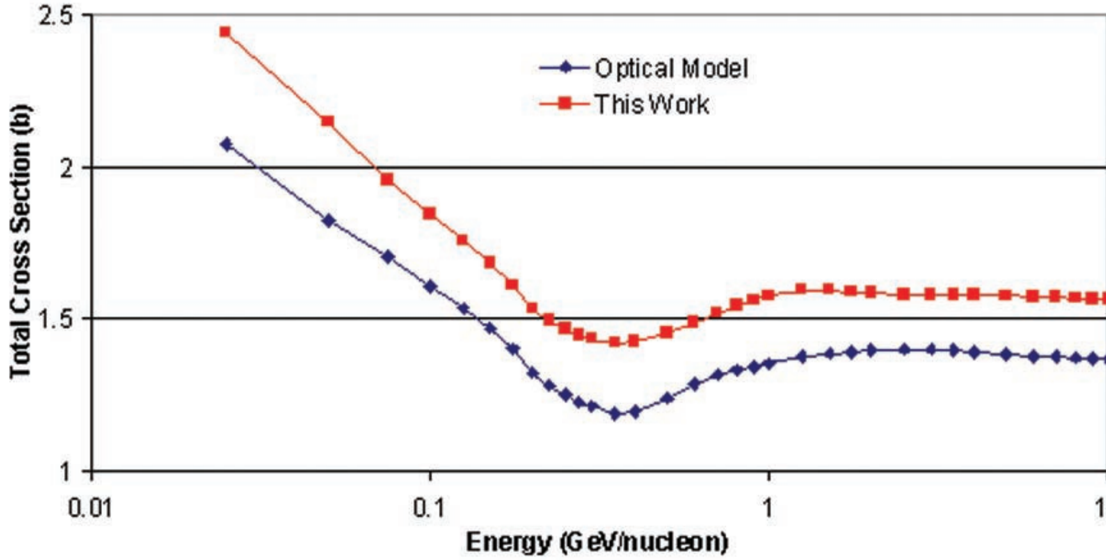


Figure 1. Total cross sections for carbon – carbon collisions as a function of energy.

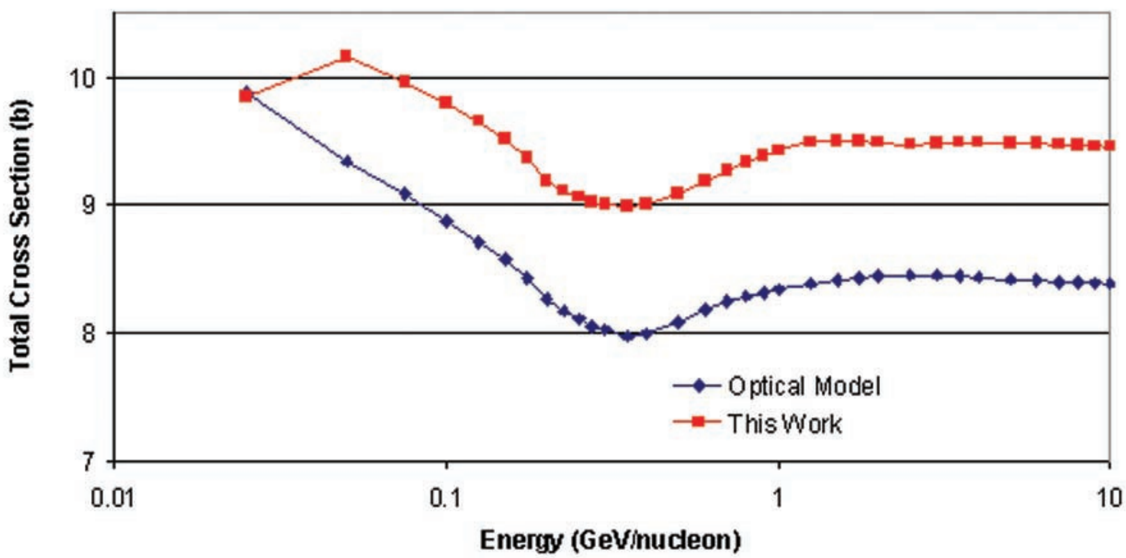


Figure 2. Total cross sections for iron – lead collisions as a function of energy.

sections exhibit strong energy dependence, especially at energies lower than ~1 GeV/nucleon. Hence, simple energy independent formulas or parameterizations, which are sometimes used in the literature, are likely to be inaccurate. The formalism represented by the above equations has been incorporated into a FORTRAN module for inclusion in the HETC/HEDS code system.

**2. Heavy Ion Fragmentation.** At present there is no one (single) event generator capable of predicting the directions and energies of all secondary particles produced in a fragmentation or spallation reaction, within a reasonable period of time, for all combinations of projectile ion, target nucleus and incident particle energy present in the GCR spectrum. Most of the models used in present day heavy ion transport codes predict inclusive cross sections (total yields) of each fragment produced in the collision. Several models have been developed for predicting the fragmentation yields (total cross sections) for secondary particles created by the breakup of a heavy-ion projectile striking a target nucleus[12-14] for space radiation transport applications. Accurate cross sections for heavy fragment production are produced by the optical potential fragmentation model of Townsend and collaborators[14]. However, this model is still under development and cannot be used at present to generate yields of nucleons and light ions. This same shortcoming exists with the semi-empirical parameterization of Silberberg and Tsao[13].

Perhaps the best model for this purpose, currently described in the literature, is the NUCFRG2 model developed at NASA Langley Research Center.[12] It accounts for all the yields of secondary light ions and heavy ion fragments produced by a nucleus-nucleus collision. NUCFRG2 is currently used to generate fragmentation databases for the publicly released 1-D deterministic GCR transport code HZETRN developed at NASA Langley.[15] Table 1 displays representative isotope production results for 1 GeV/nucleon carbon colliding with carbon targets. Note that summing these cross sections gives a result that is greater than the total reaction cross section for the collision. This is because the cross sections are inclusive, which means that the results for light ions ($Z \leq 2$) include multiplicity effects. Corrections to the multiplicities resulting from the inclusive nature of the calculations must be incorporated since exclusive cross sections are needed. The isotope yields predicted by the projectile fragmentation models discussed above are in the form of total cross sections or yields. Hence, they are invariant with respect to reference frame. Therefore, cross sections for producing target fragments can be obtained by interchanging the projectile and target nuclei at the same kinetic energy per nucleon.

Table 1. NUCFRG2 Output for 1 GeV/nucleon carbon-carbon collisions

| Fragment Charge | Fragment Mass | Production Cross Section (mb) | Fragment Charge | Fragment Mass | Production Cross Section (mb) |
|---|---|---|---|---|---|
| 6 | 11 | 5.290E+01 | 3 | 6 | 2.862E+01 |
| 6 | 10 | 3.538E-01 | 3 | 5 | 0.000E+00 |
| 6 | 9 | 2.730E-03 | 3 | 4 | 0.000E+00 |
| 6 | 8 | 2.300E-06 | 3 | 3 | 0.000E+00 |
| 5 | 11 | 5.312E+01 | 3 | 2 | 0.000E+00 |
| 5 | 10 | 5.457E+01 | 2 | 9 | 4.610E-06 |
| 5 | 9 | 3.074E+00 | 2 | 8 | 3.350E-05 |
| 5 | 8 | 1.600E-02 | 2 | 7 | 0.000E+00 |
| 5 | 7 | 0.000E+00 | 2 | 6 | 3.674E-01 |
| 5 | 6 | 3.750E-06 | 2 | 5 | 0.000E+00 |
| 4 | 11 | 0.000E+00 | 2 | 4 | 1.512E+02 |
| 4 | 10 | 3.299E+00 | 2 | 3 | 1.173E+01 |
| 4 | 9 | 1.315E+01 | 2 | 2 | 0.000E+00 |
| 4 | 8 | 3.452E+00 | 2 | 1 | 0.000E+00 |
| 4 | 7 | 1.895E+01 | 2 | 0 | 0.000E+00 |
| 4 | 6 | 7.850E-02 | 1 | 7 | 0.000E+00 |
| 4 | 5 | 0.000E+00 | 1 | 6 | 3.330E-05 |
| 4 | 4 | 0.000E+00 | 1 | 5 | 0.000E+00 |
| 3 | 11 | 0.000E+00 | 1 | 4 | 0.000E+00 |
| 3 | 10 | 2.520E-03 | 1 | 3 | 0.000E+00 |
| 3 | 9 | 3.420E-02 | 1 | 2 | 6.189E+01 |
| 3 | 8 | 1.061E-01 | 1 | 1 | 4.479E+03 |
| 3 | 7 | 2.053E+01 | 1 | 0 | 0.000E+00 |

Since secondary particle directions of travel must also be specified, we use momentum distribution models to select the directions and energies of the collision fragments. At high energies secondary ion fragments of GCR particle interactions typically travel in the direction of the incident ion with some slight angular dispersion and momentum loss resulting from the momentum transfers that occur during the collision. These fragment momentum distributions, which are experimentally found to be Gaussian in shape, can be obtained from phenomenological models such as those due to Tripathi and Townsend[16] or due to Tsao and collaborators.[17] The Tsao parameterization is used in this work. It is more complete than the other model in that it estimates momentum components in both the parallel and transverse directions as well as the widths of these momentum distributions. Typical results for two different fragments resulting from a 1 GeV/nucleon carbon - carbon collision are shown below in Table 2. Note that the model presents momentum distribution in both the laboratory frame (3-D Analysis) and in the projectile nucleus rest frame (Beam Analysis). Symbols used in the table include KE (kinetic energy), S_KE (standard deviation

Table 2. Summary of Momentum Output from Tsao et al Model[17]

| SYSTEM: (12, 6) + (12, 6) --> (8, 4) + X. | | SYSTEM: (12, 6) + (12, 6) --> (4, 2) + X. | |
|---|---|---|---|
| Projectile spallation product: | | PROJECTILE SPALLATION PRODUCT: | |
| *** 3-D Analysis ***: | | *** 3-D ANALYSIS ***: | |
| Nominal KE [lab]: | 1.0000E+03 MeV/ nucleon | Nominal KE [lab]: | 1.0000E+03 MeV/ nucleon |
| Estimated KE: | 9.7786E+02 MeV/ nucleon | Estimated KE: | 9.6210E+02 MeV/ nucleon |
| Estimated KE loss: | 2.2139E+01 MeV/ nucleon | Estimated KE loss: | 3.7905E+01 MeV/ nucleon |
| Estimated KE loss (%): | 2.21E+00 | Estimated KE loss (%): | 3.79E+00 |
| Estimated S_KE (%): | 5.35E+00 | Estimated S_KE (%): | 8.72E+00 |
| *** Beam Analysis ***: | | *** BEAM ANALYSIS ***: | |
| <PII> in Proj. Frame: | -6.2217E+01 MeV/c | <PII> in Proj. Frame: | -7.3067E+01 MeV/c |
| S_PII in Proj. Frame: | 1.9738E+02 MeV/c | S_PII in Proj. Frame: | 1.9738E+02 MeV/c |
| S_Ppe in Proj. Frame: | 3.9476E+02 MeV/c | S_Ppe in Proj. Frame: | 3.9476E+02 MeV/c |
| <BII> in Proj. Frame: | -8.33E-03 | <BII> in Proj. Frame: | -1.56E-02 |
| Estimated KE loss: | 1.1932E+01 MeV/ nucleon | Estimated KE loss: | 1.8944E+01 MeV/ nucleon |
| Estimated KE loss (%): | 1.19E+00 | Estimated KE loss (%): | 1.89E+00 |

of KE), <Pll> (mean value of momentum parallel to beam), S_Pll (standard deviation of Pll), S_Ppe (standard deviation of the transverse component of momentum; note that the transverse momentum in the projectile rest frame is zero), and <Bll> (longitudinal component of the relative velocity as a fraction of the speed of light). The Tsao model is currently being used to generate a database, which will be incorporated into a fragmentation module in the HETC/HEDS code, either in tabular or parameterized form.



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**3. Nucleon Production.** A model for neutron production in high-energy heavy ion collisions by Cucinotta, Townsend, and Wilson[18] is currently being developed under a separate project funded by the NASA Microgravity Materials Science Program. The model is also capable of predicting proton emission in high-energy heavy ion collisions as well. Work on this new nucleon production model is nearly complete. When completed it will be used to generate nucleon emission spectra (energy and angle) for the HETC/HEDS code system.

## IV. Conclusions

The current status of developments in extending the HETC code to transport galactic cosmic ray heavy ions for space radiation transport and shielding applications has been reviewed. Efforts to develop modules describing the nuclear interactions of these ions, and their transport through matter have been presented. Sample results for total cross sections and momentum distributions were shown. Future work needed to complete the development of the HETC/HEDS code system was also discussed.

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