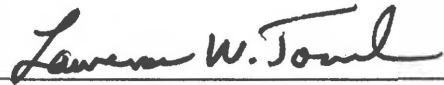


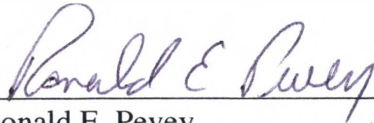
To the Graduate Council:

I am submitting herewith a dissertation written by Thomas Martin Miller entitled "Comprehensive Cross Section Database Development for Generalized Three Dimensional Radiation Transport Codes." I have examined the final paper copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Nuclear Engineering.

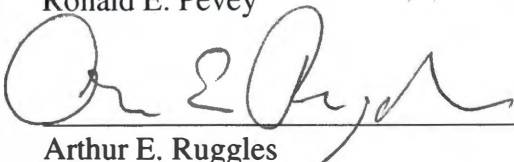


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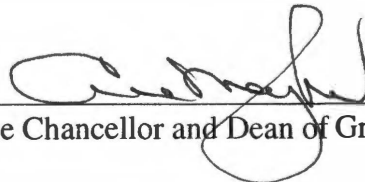


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Acceptance for the Council:



Vice Chancellor and Dean of Graduate Studies

**COMPREHENSIVE CROSS SECTION DATABASE
DEVELOPMENT FOR GENERALIZED THREE
DIMENSIONAL RADIATION TRANSPORT CODES**

**A Dissertation
Presented for the
Doctor of Philosophy
Degree
The University of Tennessee, Knoxville**

**Thomas Martin Miller
December 2004**

Thesis
2004b
.M55

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DEDICATION

For my loving wife, Allison

Thank you to my mother, Jane

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ABSTRACT

To correctly specify the composition and spectra of heavy ion radiation fields, such as those encountered in space radiation protection studies, as they are transported through shielding, accurate values of the total, elastic scattering, and reaction cross sections, spectral distributions and angular distributions of all emitted particles (nucleons, light ions and heavy ions) from the nuclear interactions of propagating high energy heavy ion (HZE) particles with target nuclei are required. For space radiation protection studies, this means that double-differential (energy and angle) isotope production cross sections must be known for all stable nuclear isotopes with mass numbers from 1 to about 60 colliding with any target nucleus at energies from tens of MeV per nucleon up to several GeV per nucleon. With this cross section database, transport codes would be able to transport nearly any radiation field that man or machine might be exposed to in space or otherwise. This database is the first high speed comprehensive database suitable for three dimensional radiation transport. Once the comprehensive database was completed, it was incorporated into HETC to create a generalized, three dimensional radiation transport code, HETC-HEDS for space applications.

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I. INTRODUCTION

For years NASA has investigated space radiation protection of astronauts and electronics. This research has included the creation of nuclear interaction models for the particles found in the space environment, transport codes that use these models to describe the changes in the space radiation fields as they penetrate shielding, and materials research to determine the best shield materials for these particles and even to create new shield materials for these particles. This research has traditionally differed from that done for terrestrial radiation protection because of the different particle species and energies of those particles present in their respective radiation environments. In recent years, as new higher power accelerator systems have been built and the interest in charged particle radiotherapy has grown, research on terrestrial and space radiation protection has converged. In spite of this convergence of interest the amount of research concerning radiations like those in the ambient space field increased only slightly. However, now that the United States has decided to return to the moon and to further explore Mars, interest in this research area has increased even more, and in turn, NASA is increasing the amount of research being carried out in this field. NASA realizes that for human exploration of Mars to be successful NASA's space radiation protection capabilities need to be improved. This dissertation is just one aspect of NASA's work that has sprouted from its new focus on space radiation protection.

Justification & Originality

To correctly specify the composition and spectra of heavy ion radiation fields, such as those encountered in space radiation protection studies, as they are transported through shielding, accurate values of the total, elastic scattering, and reaction cross sections, spectral distributions and angular distributions of all emitted particles (nucleons, light ions and heavy ions) from the nuclear interactions of propagating high energy heavy ion (HZE) particles with target nuclei are required. For space radiation protection studies, this means that double-differential (energy and angle) isotope production cross sections must be known for all stable nuclear isotopes with mass numbers from 1 to about 60 colliding with any target nucleus at energies from tens of MeV per nucleon up to several GeV per nucleon. Clearly, measuring all of these thousands of cross sections and distributions is virtually impossible due to the sheer number of measurements that would be required. Hence, the databases necessary to properly describe these reactions must be obtained using nuclear models.

There are several radiation transport codes that transport high energy nucleons, light ions, heavy ions, or some combination of them. At the time this research was started, none transported all of these particles in more than one dimension. Since the beginning of this research similar work has been undertaken in the transport codes PHITS (Iwase, Niita, and Nakamura) and FLUKA (Fasso' et. al.). In order to make a comprehensive tool for space applications that transports all of these particles, with a wide range of energies and

in three spatial dimensions, the database described above is needed, particularly for light and heavy ions. With this database, transport codes would be able to transport nearly any radiation field that man or machine might be exposed to in space or otherwise. It would be invaluable for space radiation protection, in low earth orbit or deep space, and it could be used for terrestrial purposes as well, such as accelerator shielding or charged particle radiotherapy.

The new and innovative feature of this work is that a comprehensive cross section database for generalized three dimensional radiation transport has been developed. This database contains total, elastic scattering, and reaction cross sections along with secondary particle production distributions for these reactions. The secondary particle production distributions are fully energy and angle dependent. This database is the first high speed comprehensive database suitable for three dimensional radiation transport. Once the comprehensive database was completed, it was incorporated into HETC (Gabriel et. al.) to create a generalized, three dimensional radiation transport code, HETC-HEDS (Townsend, Miller, and Gabriel) for space applications.

Space Radiation Environment

The main sources of ionizing radiation in the space environment are the trapped radiation in the Van Allen belts, consisting mainly of protons in the inner belt and electrons in the outer belt, solar energetic particles, produced by events such as coronal mass ejections

and associated phenomena on the Sun, and the galactic cosmic ray (GCR) background, composed of all naturally-occurring elements.

Van Allen Belts

The earth is protected from much of the radiation in space by its own magnetic field. However, this magnetic field can capture charged particles and keep them trapped in belts surrounding the earth. These trapped particles consist of electrons and protons, and the belts that they form are called the Van Allen Belts, named for the scientist that discovered them. Figure 1.1 gives an idea of these particles energies and distances from the earth.

The belts' spatial distribution is determined by the magnetic field of the Earth. Therefore, the belts are subject to deformation by solar activity. In general the particles in the belts are located at higher altitudes at the equator and lower altitudes at the poles. However, there is a phenomenon referred to as the South Atlantic Anomaly where the belts are closer to the earth's surface than at any other points along the same line of latitude. The particles in the trapped belts come from a variety of sources. The protons in the trapped belts likely come from fragmentation events with the GCRs and the Earth's atmosphere and from the Sun. The electrons in the trapped belts can come from the Sun and from stripping reactions of GCRs, which are not fully ionized, as they enter the earth's atmosphere (Townsend).

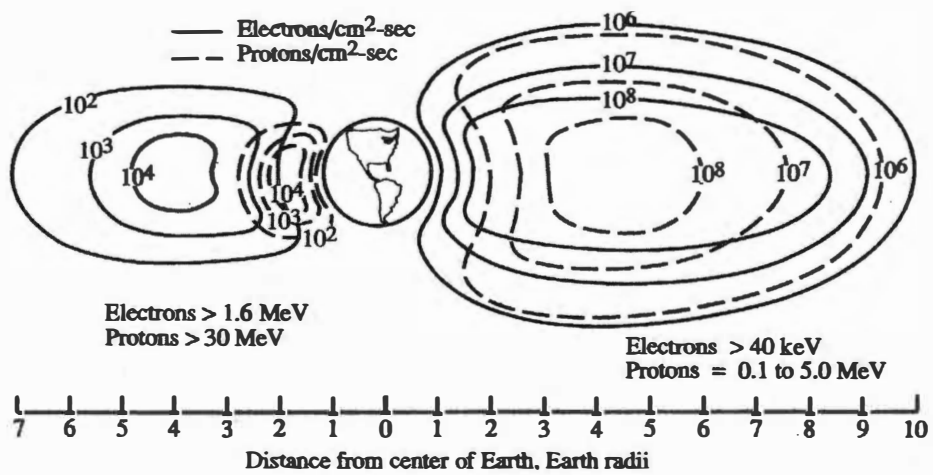


Figure 1.1: Van Allen Belts (Parker and West)

Solar Particle Events

The Sun, which plays a major role in life on Earth, plays a major role in the space radiation environment. As was previously stated, the sun can affect the trapped radiation belts, and it can also affect the GCRs, which will be discussed next. More importantly the sun is also a major source of radiations in the space environment. These radiations are energetic particles that are emitted from solar flares and coronal mass ejections, which are collectively known as solar particle events (SPEs). The species of these particles include electrons, protons, alpha particles, and other heavy ions, and their energies extend over a broad range. A SPE can occur at anytime, but typically more occur during the maximum of the approximately 11 year solar cycle. The duration of a SPE can be from a few hours up to several days. These last two statements point to some serious concerns about SPEs in relation to space radiation protection. SPE occurrences and durations are very hard to predict. That being said, it is worthwhile to point out that most solar particle events are not a major concern. Usually, the energies and/or fluxes of an SPE are too low to be a major concern, or the particles emitted by the event may not travel in a direction that is a concern for space radiation protection. On average about 2 SPEs per solar cycle are large enough and have the proper orientation to be a concern for space radiation protection. Of the particle species listed before that are present in SPEs only protons are a major concern and sometimes alpha particles. The fluxes of the other particles are typically much less than those of protons. On the other hand the fluxes of protons and sometimes alpha particles can be orders of magnitude higher than in the GCR

background. Figure 1.2 shows the integral proton fluence $\left(\int_{E'}^{\infty} \Phi(E) dE \right)$ of four large SPEs. The SPEs shown in Figure 1.2 each have some historical significance. However, it must be pointed out that there may more important SPEs that predate our ability to measure their fluences. The February 1956 event had the hardest spectrum, the November 1960 event had a significant alpha particle component, the August 1972 event had the largest dose, and the November 1989 event had the largest fluence (Townsend).

Galactic Cosmic Rays

The final portion of the space radiation environment is the galactic cosmic ray background. The GCRs are ions that originate from outside our solar system, and are thought to come from super nova. However, their actual origins are unknown. The particle species present in the GCRs include all naturally occurring isotopes from protons to uranium, but also include beta particles. The energies of the GCRs have a very broad range and cover several orders of magnitude with peaks around 1 GeV per nucleon. Figure 1.3 shows the fluence of GCR ions at 2 GeV per nucleon relative to the fluence of silicon at 2 GeV per nucleon. Several peaks in Figure 1.3 are labeled pointing out some of the more important ions in the GCR spectrum, which include H, He, C, O, Si, and Fe. In reality 98 percent of the GCRs are baryons while the remaining 2 percent are electrons. Of that 98 percent, 87 percent are protons, 12 percent are alpha particles, and the remaining 1 percent consists of other heavier ions. The intensity of the GCRs seen on

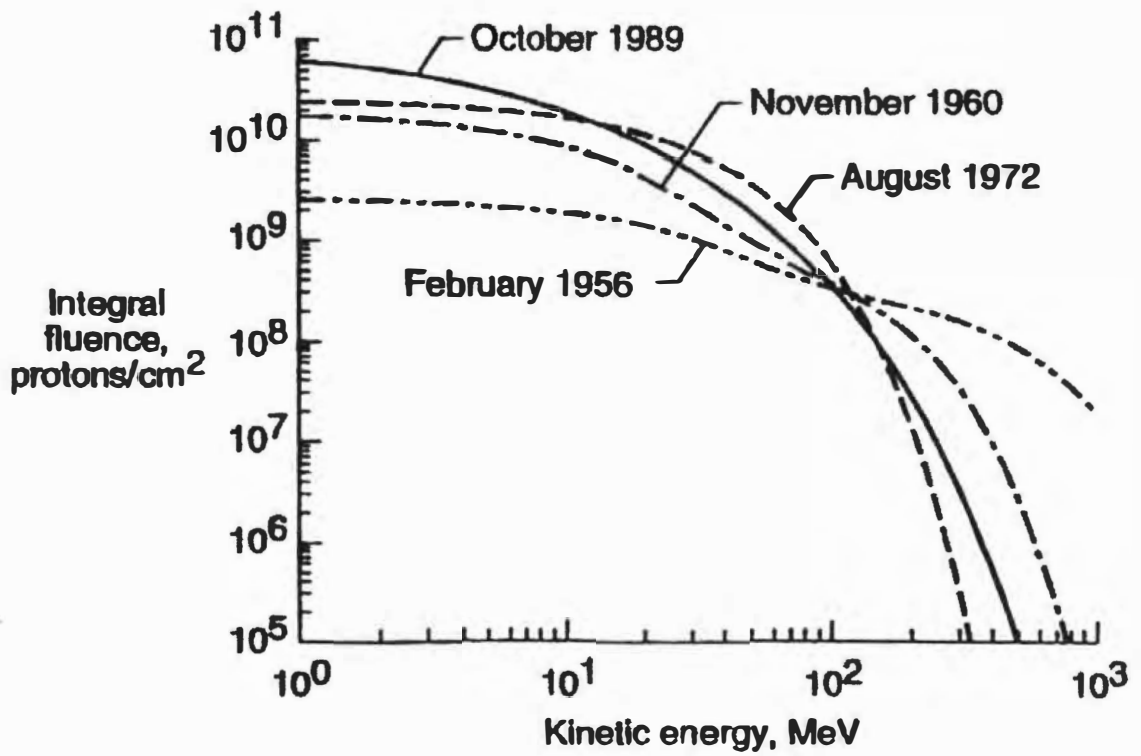


Figure 1.2: Integral Proton Fluence of Four Large SPEs (Townsend)

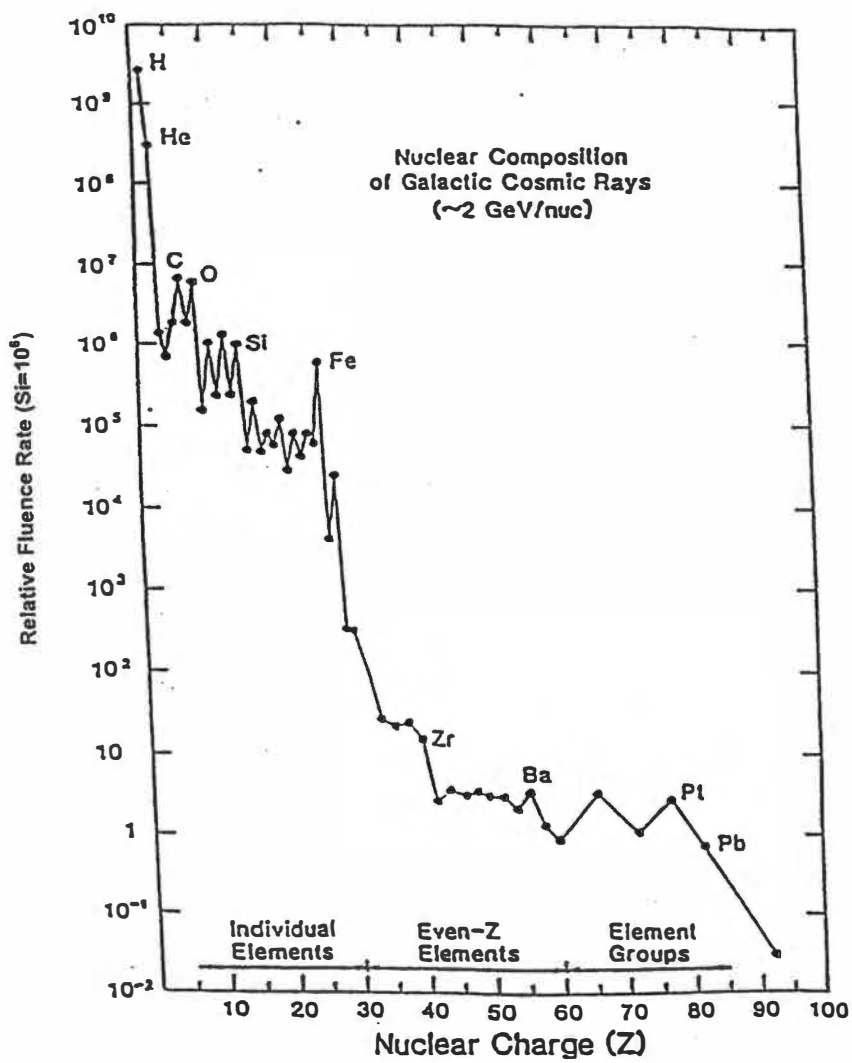


Figure 1.3: GCR Fluence at 2 GeV per Nucleon (Mewaldt)

Earth or in Low Earth Orbit (LEO) is affected by the solar cycle because solar activity affects the earth's magnetic field. The GCR spectrum is at a minimum during solar maximum and at a maximum during solar minimum. This difference in the spectrum is primarily due to the deflection of low energy ions by the magnetic fields associated with solar wind plasma. The GCR intensity below 1 GeV per nucleon can fall about an order of magnitude between solar minimum and solar maximum (Townsend).

Charged Particle Transport

Now that the space radiation environment has been clearly defined one must address how the movement and interaction of these radiations are modeled. As was stated before there currently exists several radiation transport codes that transport high-energy nucleons, light ions, heavy ions, or some combination of them. When this research began, none transported all of these particles in more than one dimension; subsequently work has begun on PHITS and FLUKA using quantum mechanical models. Some examples of these are discussed next. Two codes developed at NASA's Langley Research Center (LaRC) are HZETRN (Wilson et. al. 1995) and BRYNTRN (Wilson et. al. 1989). BRYNTRN transports neutron, protons, deuterons, tritons, helions, and alphas all in one dimension. This code was created primarily to perform dose calculations due to SPEs. HZETRN is also a one dimensional transport code, but in addition to the nucleons and light ions BRYNTRN transports heavy ions. HZETRN is well suited to perform dose calculations due to the GCR background. BRYNTRN and

HZETRN are both deterministic codes, and apply an analytic solution to the one dimensional Boltzmann equation. In general a one dimensional treatment for the charged particles works fairly well, but does a very poor job for neutron transport. To overcome this obstacle it is not uncommon for people to perform dose calculations where the SPE or GCR spectrum has been broken into individual neutrons and protons. With this all nucleon source three dimensional high energy transport codes, such as HETC or MCNPX (Waters) can be used. HETC and MCNPX both apply Monte Carlo methods to perform these calculations. HETC will transport neutrons, protons, muons, and pions, and MCNPX will transport these particles plus all the remaining mesons, leptons, and the light ions included in BRYNTRN. While this approximate all nucleon source will allow one to calculate an upper limit on the dose it does not properly account for the slowing down of the individual nucleons when they were part of an ion. This is particularly a problem for neutrons.

HETC and MCNPX both perform a “random walk” to perform these transport calculations, so the theory behind them is not much different from neutral particle transport. One obvious difference is that the particles are charged, not neutral, but this can be handled in much the same way electron transport in various codes is handled. So the major differences are the interaction cross sections, particle production, and range and stopping power data. In order to discuss these things in the context of a transport code a discussion of the theory applied in BRYNTRN and HZETRN is useful.

Begin by defining a sphere of material with known macroscopic interaction cross sections. This sphere has a radius δ , its center is located at the point $\vec{x}$, the flux of particles of type j passing through the center and entering the sphere through a differential surface area, $\delta^2 d\vec{\Omega}$, in direction $\vec{\Omega}$ and energy E is

$$\phi_j(\vec{x} - \delta\vec{\Omega}, \vec{\Omega}, E) \delta^2 d\vec{\Omega}, \quad (1.1)$$

and the flux of particles of type j leaving the sphere through a similar differential surface area in the same direction with the same energy is

$$\phi_j(\vec{x} + \delta\vec{\Omega}, \vec{\Omega}, E) \delta^2 d\vec{\Omega}. \quad (1.2)$$

This system can be seen graphically in Figure 1.4. Now in order to create a balance of type j particles entering and leaving the sphere the gains and losses of type j particles in the sphere must be accounted for. Gains of type j particles are defined as the production of type j particles from nuclear and atomic interactions in the direction $\vec{\Omega}$ with energy E from the interactions of type k particles traveling in the direction $\vec{\Omega}'$ with energy E' . These gains can be shown mathematically to be:

$$\delta^2 d\vec{\Omega} \int_{-\delta}^{\delta} dl \sum_k \int \sigma_{jk}(\vec{\Omega}' \rightarrow \vec{\Omega}, E' \rightarrow E) \phi_k(\vec{x} + l\vec{\Omega}, \vec{\Omega}', E') d\vec{\Omega}' dE'. \quad (1.3)$$

It is worth pointing out here that the macroscopic cross section $\sigma_{jk}(\vec{\Omega}' \rightarrow \vec{\Omega}, E' \rightarrow E)$ is inclusive of all interactions that produce particles of type j with the desired direction and energy from any particle of type k . Losses of type j particles occur when type j particles traveling in the direction $\vec{\Omega}$ with energy E have an interaction through which the particle's species, direction, energy, or some combination of those changes. These losses

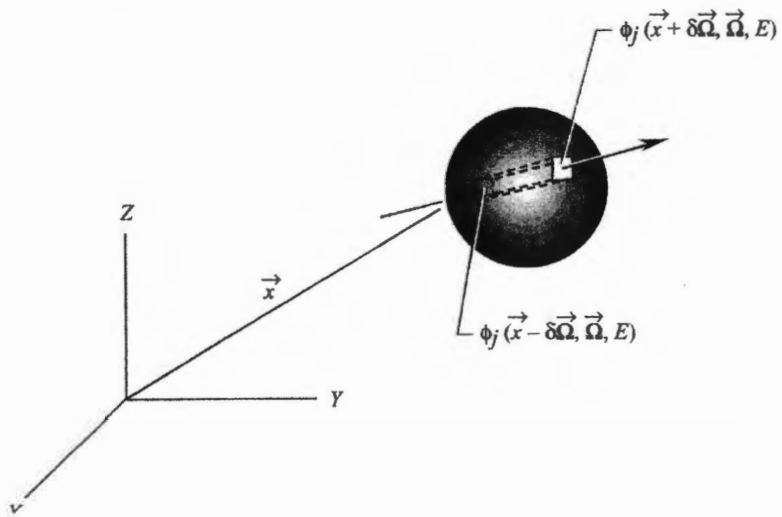


Figure 1.4: Sphere of Radius δ at Position $\vec{x}$ (Wilson et. al., p. 75, 1995)

can be shown mathematically to be:

$$\delta^2 d\vec{\Omega} \int_{-\delta}^{\delta} dl \sigma_j(E) \phi_j(\vec{x} + l\vec{\Omega}, \vec{\Omega}, E). \quad (1.4)$$

Now a balance equation for particles of type j can be written for the sphere as a fix control volume, which will have the form:

outflow – inflow = gains – losses, or

$$\begin{aligned} & \phi_j(\vec{x} + \delta\vec{\Omega}, \vec{\Omega}, E) \delta^2 d\vec{\Omega} - \phi_j(\vec{x} - \delta\vec{\Omega}, \vec{\Omega}, E) \delta^2 d\vec{\Omega} = \\ & \delta^2 d\vec{\Omega} \int_{-\delta}^{\delta} dl \sum_k \int \sigma_{jk}(\vec{\Omega}' \rightarrow \vec{\Omega}, E' \rightarrow E) \phi_k(\vec{x} + l\vec{\Omega}, \vec{\Omega}', E') d\vec{\Omega}' dE' . \\ & - \delta^2 d\vec{\Omega} \int_{-\delta}^{\delta} dl \sigma_j(E) \phi_j(\vec{x} + l\vec{\Omega}, \vec{\Omega}, E) \end{aligned} \quad (1.5)$$

In order to simplify equation (1.5) one can make a Taylor expansion of the flux of type j particles, drop terms of order δ^4 and higher, divide by the spherical volume, and rewrite the equation as:

$$\begin{aligned} & \vec{\Omega} \cdot \vec{\nabla} \phi_j(\vec{x}, \vec{\Omega}, E) = \\ & \sum_k \int \sigma_{jk}(\vec{\Omega}' \rightarrow \vec{\Omega}, E' \rightarrow E) \phi_k(\vec{x}, \vec{\Omega}', E') dE' d\vec{\Omega}' - \sigma_j(E) \phi_j(\vec{x}, \vec{\Omega}, E). \end{aligned} \quad (1.6)$$

Equation (1.6) is also known as the time independent Boltzmann equation for particles in a tenuous gas.

Next, consider the macroscopic cross sections in equation (1.6). These cross sections can be separated into 3 pieces, the atomic, elastic, and reaction pieces. The atomic cross section describes the interactions of particles with atomic electrons. These interactions only result in slowing the particle down, i.e. changing its energy. The elastic cross

section describes the nuclear elastic scattering that these particles undergo. Elastic scattering interactions change the energy and/or direction of the particle. The reaction piece actually describes all other nuclear interactions the particle may experience. These include inelastic scattering, fragmentation, spallation, and fission. All of these interactions can not only change the energy and direction of the particles but also the particle species. This is represented mathematically in equation (1.7):

$$\sigma_j(E) = \sigma_j^{atomic}(E) + \sigma_j^{elastic}(E) + \sigma_j^{reaction}(E) = \sigma_j^{atomic}(E) + \sigma_j^{nuclear}(E). \quad (1.7)$$

Looking more closely at the atomic cross section, and the fact that these interactions only change the energy of the particle, it is clear that the energy lost by the scattered particle is due to excitation of the struck atom, therefore the new energy is:

$$E = E' - \varepsilon_n, \quad (1.8)$$

where ε_n is the excitation energy of the n^{th} atomic level. Then the atomic cross section can be written as:

$$\sigma_{jk}^{atomic}(\vec{\Omega}' \rightarrow \Omega, E' \rightarrow E) = \sum_n \sigma_{jn}^{atomic}(E) \delta(\vec{\Omega} \cdot \vec{\Omega}' - 1) \delta_{jk} \delta(E' - \varepsilon_n - E). \quad (1.9)$$

Separating the cross sections in equation (1.6), using equation (1.9) to represent the atomic cross sections, and performing a Taylor expansion (similar to the one done previously) on the term $\sigma_{jn}^{atomic}(E) \phi_j(\vec{x}, \vec{\Omega}, E' - \varepsilon_n)$ the Boltzmann equation can be written as:

$$\begin{aligned} \vec{\Omega} \cdot \vec{\nabla} \phi_j(\vec{x}, \vec{\Omega}, E) - \frac{\partial}{\partial E} [S_j(E) \phi_j(\vec{x}, \vec{\Omega}, E)] + \sigma_j^{nuclear}(E) \phi_j(\vec{x}, \vec{\Omega}, E) = \\ \sum_k \int \sigma_{jk}^{nuclear}(\vec{\Omega}' \rightarrow \vec{\Omega}, E' \rightarrow E) \phi_k(\vec{x}, \vec{\Omega}', E') d\Omega' dE' \end{aligned} \quad (1.10)$$

Note that in equation (1.10) all of the atomic scattering terms have disappeared and a new term has been introduced, $S_j(E)$, which is the stopping power. The stopping power is the average energy loss of a charged particle per unit path length, and in general can be expressed as:

$$S_j(E) \equiv \sum_n \sigma_{jn}^{atomic}(E) \epsilon_n . \quad (1.11)$$

Replacing the atomic interaction cross section with the stopping power is referred to as the continuous slowing down approximation. However, equation (1.11) does not provide a practical method for calculating the stopping power. This is done by using the well known Bethe form of the stopping power:

$$S(E) = \frac{4\pi e^4 N Z_t^2 Z_p^2}{mv^2} \left[\ln \left(\frac{2mv^2}{(1 - \beta^2) I_t} \right) - \beta^2 - \frac{C}{Z_t} \right], \quad (1.12)$$

where Z_t and Z_p are the atomic charge of the target and projectile, respectively, m is the electron mass, N is the target number density, v is the projectile velocity, I_t is the mean excitation energy of the atomic electrons, β is the relativistic velocity (i.e. v/c where c is the speed of light), and C is a shell correction term to account for tightly bound inner shell electrons.

In the space radiation environment a few more assumptions can be applied to equation (1.10). First, the kinetic energy of the projectiles are usually high enough that it is a fair approximation to assume that projectile fragments will continue in the same direction and with the same energy per nucleon as the projectile. This is the straight ahead approximation and allows for the problem to be reduced to one dimension. Next, target

and projectile fragment contributions to the flux can be separated, and target fragment contributions can be treated as local energy deposition because their kinetic energies are much less than projectile fragments. Therefore, the straight ahead approximation of the Boltzmann equation is:

$$\left[\frac{\partial}{\partial x} - \frac{\partial}{\partial E} S_j(E) + \sigma_j^{nuclear}(E) \right] \phi_j(x, E) = \sum_{k>j} \int_E^\infty \sigma_{jk}^{nuclear}(E' \rightarrow E) \phi_k(x, E') dE'. \quad (1.13)$$

HZETRN and BRYNTRN perform shielding calculations using the straight ahead approximation of the Boltzmann equation by implementing the method of characteristics. However, equation (1.13) is not the exact equation that is solved. A transformation is made from position and energy space to range space:

$$\begin{aligned} \eta_j &\equiv x - R_j(E) \\ \xi_j &\equiv x + R_j(E) \end{aligned} \quad (1.14)$$

where $R_j(E)$ is the range of particle type j with energy E given by:

$$R_j(E) = \int_0^E \frac{dE'}{S_j(E')}. \quad (1.15)$$

This mapping reduces the Boltzmann equation to the form:

$$\left[2 \frac{\partial}{\partial \eta_j} + \sigma_j(E) \right] \phi_j(\eta_j, \xi_j) = \sum_k \sigma_{jk}(E' \rightarrow E) \left(\frac{Z_j^2 A_k}{A_j Z_k^2} \right) \phi_j(\eta_k, \xi_k). \quad (1.16)$$

Once the solution to equation (1.16) has been found it can be mapped back into position and energy space from range space via the reverse of the transform defined in equation (1.14). The differential fluence solution can be written as:

$$\begin{aligned} \psi_j(x+h, R_j(E)) &\approx e^{-\sigma_j(E)h} \psi_j(x, R_j(E)+h) \\ &+ e^{-\sigma_j(E)h} \int_0^h dx \int_{R_j(E)}^{\infty} \sigma_{jk}(R'_j(E')+z \rightarrow R_k(E)+z) \psi_k(x, R'_k(E')+h) \end{aligned} \quad (1.17)$$

where $\psi_j(x, R_j(E)) = S_j(E)\phi(x, E)$. Finally, the differential fluence of particle type j can be found by numerically integrating equation (1.17) by making steps of size h from x=0 to the desired thickness of shield material.

All of this material has been a summary of the information found in the references previously given for HZETRN and BRYNTRN, and in NASA Reference Publication 1257 entitled, "Transport Methods and Interactions for Space Radiations" (Wilson et. al. 1991).

Definition of Terms

In traditional nuclear engineering the transport of particles is almost exclusively limited to neutrons and photons with spectra from fission power reactors, i.e. energies less than or equal to 20 MeV. In this traditional setting scattering is broken into elastic and inelastic scattering. Elastic scattering occurs when two particles interact and conservation of energy after the interaction is achieved by just dealing with the kinetic energy of the particles. As an example, this is the type of collision that occurs between two billiard balls. Inelastic scattering is similar to elastic scattering in that the particles do not change species, but with inelastic scattering excitation of the particles must also be

considered in the conservation of energy. Another term used in a traditional nuclear engineering setting is absorption. Absorption is when a target absorbs a projectile. Subsequently that target may or may not become excited. If the target does become excited it will undergo some process to rid itself of that excitation energy, for example the target may emit a particle that is a different species as the projectile with a new energy and direction, or the target may undergo fission.

In this work, which primarily deals with high energy charged particles, the terms elastic scattering, inelastic scattering, and absorption are not used in the traditional meanings of nuclear engineering. Scattering is broken into elastic and inelastic scattering, and elastic scattering still has the same definition. However, inelastic scattering is different. In this work any type of interaction other than elastic scattering is referred to as inelastic scattering. Also in this work inelastic scattering and absorption are synonymous. Another synonym of inelastic scattering and absorption, and really a better term for these interactions, is reaction. This term was used previously in the section on charged particle transport and was defined as including inelastic scattering (in traditional nuclear engineering terms), fragmentation, spallation, and fission. Therefore inelastic scattering cross sections, absorption cross sections, and total reaction cross sections in this work all refer to the same cross section.

Another term that can often lead to confusion is the word fragment. In general terms fragment(s) refers to particles that emerge from a nucleus-nucleus collision. However,

fragment can more specifically refer to the remains of the prefragment. More information is given about the prefragment and the remains of the prefragment, i.e. the fragment, in Chapter II. In this work every attempt is made to always point out when the fragment being discussed is the remains of the prefragment.

Outline of Dissertation

This chapter, chapter one, has been an introduction to the problem, the space radiation environment, charged particle transport, and has defined some terms in hopes of avoiding confusion. Chapter two serves as a literature review and gives background information about the nuclear models used in this work. Chapter three describes the event generator that was created, and chapter four discusses the new code HETC-HEDS, which was created by combining the new event generator and HETC. Chapter five shows some sample results of the event generator and HETC-HEDS. Then chapter six contains a few conclusions and suggestions for future work. After the main body of this dissertation are several appendices. Appendix A contains two parts, A-1 with additional theory concerning the heavy ion fragmentation model and A-2 with additional theory about the model for fragment kinetic energy distributions. Appendix B is a user's manual for HETC-HEDS and Plate 1 (the CD-ROM attached to this dissertation) contains the actual FORTRAN coding of the nucleus-nucleus event generator.

II. EXISTING DATABASES

Several algorithms necessary to transport particles using either stochastic or deterministic methods are already well known. What is needed to create a generalized three-dimensional radiation transport code is a comprehensive cross section database of total, elastic scattering, total reaction, and double differential particle production cross sections for virtually any colliding nuclear system.

Several cross section models currently exist that contain part of the information needed to construct a comprehensive cross section database for transport of high-energy heavy ions in three-dimensions. In their current state these cross section models are not designed to work together for a fully three-dimensional transport problem. The existing models of particular interest are:

- The heavy ion total and total reaction cross section databases for incident energies above 25 MeV/nucleon developed at NASA LaRC (Townsend, Wilson, and Bidasaria, 1983A).
- The improved total reaction cross section database, above 1 MeV/nucleon developed at NASA LaRC (Tripathi, Cucinotta, and Wilson).
- The nuclear fragmentation cross sections database for heavy ions developed at NASA LaRC (Wilson et. al., 1994).

- The total and total reaction cross section database for nucleon and deuteron interactions for incident energies above 25 MeV/nucleon developed at NASA LaRC (Townsend, Wilson, and Bidasaria, 1983B).
- The nuclear fragmentation cross sections database for alpha particles developed at NASA LaRC (Cucinotta, Townsend, and Wilson).
- The microscopic model for the estimation of energy degradation in nucleus-nucleus collisions developed at the Naval Research Laboratory (NRL) (Tsao et. al.).

Total and Total Reaction Cross Sections

Townsend, Wilson, and Bidasaria's optical potential model for total cross sections and total reaction cross sections based on quantum scattering theory gives:

$$\sigma_{tot}^{optical} = 4\pi \int_0^{\infty} \{1 - e^{[-\text{Im } \chi(\bar{b})]} \cos[\text{Re } \chi(\bar{b})]\} b db \quad (2.1)$$

and

$$\sigma_R^{optical} = 2\pi \int_0^{\infty} \{1 - e^{[-2 \text{Im } \chi(\bar{b})]}\} b db . \quad (2.2)$$

The complex phase function is:

$$\chi(\bar{b}) = -\frac{1}{2k} \int_{-\infty}^{\infty} U(\bar{b}, z) dz , \quad (2.3)$$

where

$$U(\vec{x}) = \frac{2mA_P A_T}{A_P + A_T} W(\vec{x}), \quad (2.4)$$

m is the nucleon mass in kg, A_P is the nuclear mass number of the projectile, and A_T is the nuclear mass number of the target (Townsend, Wilson, and Bidasaria, 1983A). The nucleus-nucleus optical potential including Pauli correlation effects is:

$$W(\vec{x}) = A_P A_T \int d^3 \vec{\xi}_T \rho_T(\vec{\xi}_T) \int d^3 \vec{y} \rho_P(\vec{x} + \vec{y} + \vec{\xi}_T) \tilde{f}(e, \vec{y}) [1 - \tilde{C}(\vec{y})], \quad (2.5)$$

where ρ_P is the nuclear number density distribution of the projectile nucleons in fm^{-3} , ρ_T is the nuclear number density distribution of the target nucleons in fm^{-3} , $\vec{x}$ is the position vector of the projectile in fm, $\vec{y}$ is the two nucleon relative position vector in fm, $\vec{\xi}_T$ is the collection of constituent relative coordinates for targets in fm, and e is the two nucleon kinetic energy in their center of mass frame in GeV (Townsend, Wilson, and Bidasaria, 1983A). The nuclear number density distribution for nuclei lighter than neon ($A < 20$) is:

$$\rho(r)_{T,P} = \frac{\rho_0 a^3}{8s^3} \left[1 + \frac{3\gamma}{2} - \frac{3\gamma a^2}{8s^2} + \frac{\gamma a^2 r^2}{16s^4} \right] e^{-r^2/4s^2}, \quad (2.6)$$

where ρ_0 is a normalization constant, a and γ are charge parameters given by Townsend, Wilson, and Bidasaria, and:

$$s^2 = \frac{a^2}{4} - \frac{r_p^2}{6}. \quad (2.7)$$

The nuclear number density distribution for neon and nuclei that are heavier ($A \geq 20$) is:

$$\rho(r)_{T,P} = \frac{8.8r}{\sqrt{3}} \left[\ln \left(\frac{3\beta - 1}{3 - \beta} \right) \right]^{-1}, \quad (2.8)$$

where:

$$\beta = e^{4.4r/t_c \sqrt{3}} \quad (2.9)$$

and t_c is the skin thickness of the nuclei provided by Townsend, Wilson, and Bidasaria. In equation (2.5), $\tilde{t}$ is the constituent averaged energy dependent two body transition amplitude:

$$\tilde{t}(e, \bar{y}) = -\sqrt{\frac{e}{m}} \sigma(e) [\alpha(e) + i [2\pi B(e)]^{-3/2} e^{\left[\frac{-y^2}{2B(e)}\right]}], \quad (2.10)$$

where $\alpha(e)$ is the ratio of the real part to the imaginary part of the nucleon-nucleon forward scattering amplitude, $B(e)$ is the average slope parameter of the nucleon-nucleon scattering amplitude in fm^2 , and $\sigma(e)$ is the averaged nucleon-nucleon total cross section in mb (Townsend, Wilson, and Bidasaria, 1983A). $B(e)$, $\alpha(e)$, and $\sigma(e)$ are parameters given by Townsend, Wilson, and Bidasaria. Also from equation (2.5):

$$\tilde{C} = 0.25e^{\left(\frac{-k_F^2 y^2}{10}\right)}, \quad (2.11)$$

where k_F is the fermi momentum, assumed to be 1.36 fm^{-1} , which is the value for infinite nuclear matter (Townsend, Wilson, and Bidasaria, 1983A).

The deuteron and nucleon total and total reaction cross section model created by Townsend, Wilson, and Bidasaria uses nearly the same physics as their total and total reaction cross section model for heavy ions (1983B). It is an optical potential model based on quantum scattering theory. However, it is now applied to nucleons and deuterons colliding with different nuclei. Therefore, the equations for the total and total

reaction cross sections have already been give in equations (2.1) and (2.2), respectively. One difference arises in the calculation of the complex phase function because the nucleus-nucleus optical potential given in equation (2.5) contains a Pauli blocking correction. For deuterons and nucleons the optical potential that is used contains no Pauli blocking correction (Townsend, Wilson, and Bidasaria, 1983B):

$$W(\bar{x}) = A_P A_T \int d^3 \bar{\xi}_T \rho_T(\bar{\xi}_T) \int d^3 \bar{y} \rho_P(\bar{x} + \bar{y} + \bar{\xi}_T) \bar{f}(e, \bar{y}), \quad (2.12)$$

where all the terms in equation (2.12) are the same as were defined before.

The Improved Total Reaction Cross Section

The improved semiempirical total reaction cross section developed by Tripathi, Cucinotta, and Wilson is:

$$\sigma_R^{Tripathi} = \pi r_0^2 \left(A_P^{1/3} + A_T^{1/3} + \delta_E \right)^2 \left(1 - R_c \frac{B}{E_{cm}} \right) X_m, \quad (2.13)$$

where r_0 equals 1.1 fm, E_{cm} is the colliding system center of mass energy in MeV/nucleon, and R_c a the Coulomb multiplier, which is given by the Tripathi, Cucinotta, and Wilson. B is the energy dependent Coulomb interaction barrier:

$$B = \frac{1.44 Z_P Z_T}{R}, \quad (2.14)$$

where Z_P is the atomic number of the projectile and Z_T is the atomic number of the target (Tripathi, Cucinotta, and Wilson). R is the radius for evaluating the Coulomb barrier height:

$$R = r_P + r_T + \frac{1.2(A_P^{1/3} + A_T^{1/3})}{E_{cm}^{1/3}} \quad (2.15)$$

where $r_{P,T} = 1.29 r_{rms,P,T}$ which is the equivalent hard sphere radius of the projectile or target and is given by Tripathi, Cucinotta, and Wilson. Transparency and Pauli blocking effects in the reaction cross section are taken into account by:

$$\delta_E = 1.85S + \frac{0.16S}{E_{cm}^{1/3}} - C_E + \frac{0.91(A_T - 2Z_T)Z_P}{A_T A_P}, \quad (2.16)$$

where

$$S = \frac{A_P^{1/3} A_T^{1/3}}{A_P^{1/3} + A_T^{1/3}} \quad (2.17)$$

and

$$C_E = D \left[1 - e^{\frac{-E}{T_1}} \right] - 0.292 e^{\frac{-E}{792}} \cos(0.229 E^{0.453}), \quad (2.18)$$

where E is the collision kinetic energy in MeV/nucleon and D and T_1 are parameters given by Tripathi, Cucinotta, and Wilson. Finally, the optical model multiplier is given by (Tripathi, Cucinotta, and Wilson):

$$X_m = 1 - X_1 e^{\frac{-E}{X_1 S_L}}, \quad (2.19)$$

where

$$X_1 = 2.83 - (3.1 \times 10^{-2}) A_T + (1.7 \times 10^{-4}) A_T^2 \quad (2.20)$$

and

$$S_L = 1.2 + 1.6 \left[1 - e^{\frac{-E}{15}} \right]. \quad (2.21)$$

Nuclear Fragmentation Cross Sections

The fragmentation of nuclei in this discussion is divided into two parts, first the fragmentation of nuclei with charge (Z) greater than 3 and second the fragmentation of nuclei with charge 1 and 2. These two divisions have been labeled heavy ions and light ions, respectively. The fragmentation of the heavy ions is handled by NUCFRG2 (Wilson et. al., 1994) and various other models handle the fragmentation of light ions.

Heavy Ion ($Z > 2$) Fragmentation

NUCFRG2 is a semiempirical nuclear fragmentation model that predicts nuclear fragmentation cross sections (yields) for colliding systems with a projectile charge greater than 2. The processes modeled are abrasion or knockout, the process of nuclei actually breaking apart due to a direct collision, and ablation or evaporation, which involves the decay of highly excited nuclear states by heavy particle emission. In this model a projectile nucleus, moving at relativistic speeds, collides with a stationary target nucleus. The parts of the two nuclear volumes that overlap are sheared away, due to the collision, in the abrasion part of this process. The nucleons included in the overlap region are referred to as the participants or more specifically the projectile participants

and target participants. After the collision the participants are also sometimes called the fireball. The remaining piece of the projectile (or the projectile spectator) continues on in the original direction of travel at roughly the same velocity as before the collision, however, it is left in a highly excited state. This highly excited projectile spectator rids itself of this excess energy by emission of gamma rays and/or nuclear particles; this process is the ablation portion of the collision (Townsend et. al., 1993). After the collision the projectile spectator is sometimes referred to as the prefragment, and after the ablation process is complete the remaining nucleons of the prefragment are referred to as the fragment. The target spectator is also left in an excited state and undergoes the same ablation process. A schematic of the abrasion ablation process can be seen in Figure 2.1. A detailed discussion of the abrasion ablation model and how to calculate the number of nucleons removed from the projectile due to abrasion (Δ_{abr}) and ablation (Δ_{abl}) is located in Appendix A-1. Below is a discussion of how NUCFRG2 calculates the fragmentation cross sections.

The cross section for removal of ΔN nucleons is estimated as (Wilson et. al., 1994):

$$\sigma(\Delta N) = \pi b_2^2 - \pi b_1^2, \quad (2.22)$$

where b_1 and b_2 are the two impact parameters that bracket the range of impact parameters that cause the interaction zone of the projectile to contain Δ_{abr} nucleons and the resulting excitation energy releases Δ_{abl} nucleons, at the rate of one nucleon for every 10 MeV of excitation energy, so that

$$\Delta_{abr}(b_2) + \Delta_{abl}(b_2) = \Delta N - 0.5 \quad (2.23)$$

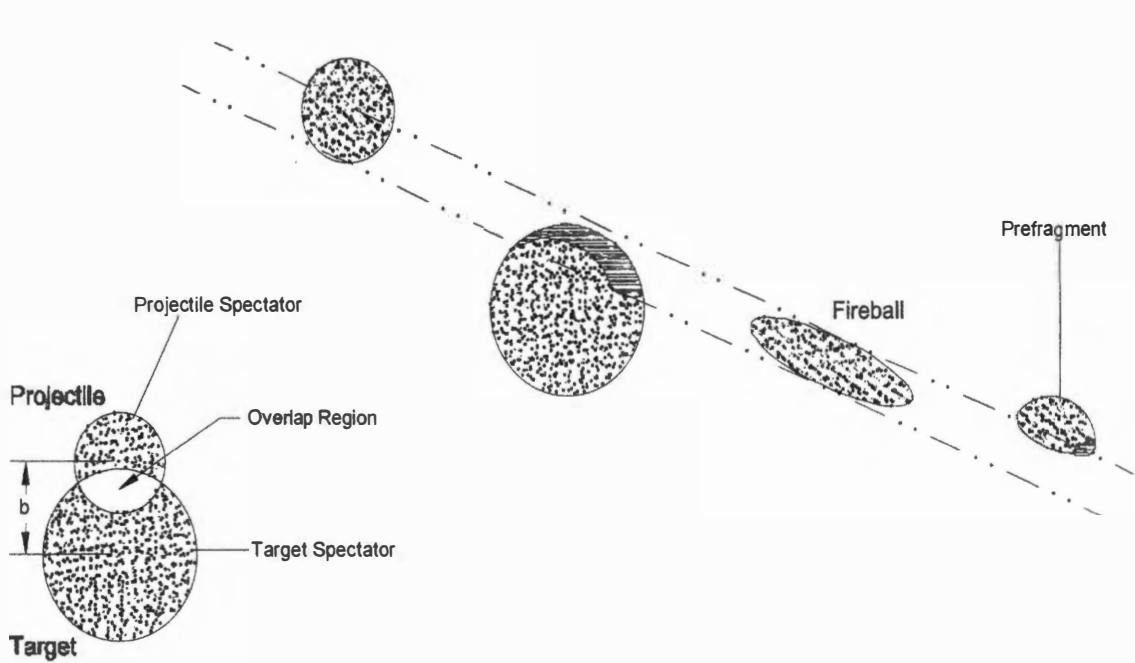


Figure 2.1: Abrasion Ablation Schematic (Stephens, 2002)

and similarly for b_1

$$\Delta_{abr}(b_1) + \Delta_{abl}(b_1) = \Delta N + 0.5. \quad (2.24)$$

The rate of particle ablation is set at one nucleon per 10 MeV of excitation energy as a crude estimate of the actual energy required to ablate a particle. This value models the actual energy needed for ablation, usually around 7 MeV per nucleon, and the remaining 3 MeV or so models excitation energy carried away by the ablated particle. Finally, the fragmentation cross section for each specific fragment isotope produced due to abrasion and ablation is:

$$\sigma(A_F, Z_F) = F_1 e^{-R \sqrt{|Z_F - S A_F + T A_F^2|}^3} \sigma(\Delta N), \quad (2.25)$$

where the factors in front of $\sigma(\Delta N)$ give the charge dispersion according to Rudstam, R is

$\frac{11.8}{A_F^D}$ and D is 0.45, S is 0.486, T is 3.8E-4, and F_1 is a normalizing faction such that

$$\sum_{Z_F} \sigma(A_F, Z_F) = \sigma(\Delta N) \quad (2.26)$$

which ensures conservation of mass number (Wilson et. al., 1994).

Light Ion ($Z \leq 2$) Fragmentation

Light ion fragmentation itself is broken into 3 pieces, which are deuteron breakup, alpha fragmentation, and Helium-3 and Triton Fragmentation.

Deuteron Breakup

The simplest projectile to determine the fragmentation products of is the deuteron because it only has one reaction channel:



Therefore, the total reaction cross section is equal to the production cross section of the deuteron's single reaction channel. Since the deuteron breakup cross section is equivalent to its total reaction cross section equation (2.13), Tripathi's improved total reaction cross section, also serves as the deuteron breakup model.

Alpha Fragmentation

Cucinotta, Townsend, and Wilson have developed a parameterization of helium-3, triton, and deuteron production due to alpha particle fragmentation on hydrogen targets. The cross section for helium-3 production is:

$$\sigma_{He-3}^{Cucinotta} = 42.5 \left[\frac{2}{1 + e^{(T_{th}-T)/6.8}} - 1 \right] \left(1 - \frac{0.51}{1 + 6.7e^{-T/34}} \right)^3, \quad (2.28)$$
$$\times \left[1 + 0.36 \sqrt{\frac{T}{520}} \right] \left(e^{(780-T)/2300} \right)$$

where T_{th} is the threshold energy for the possible fragmentation events, which are listed below in Table 2.1, and T is the kinetic energy of the projectile in units of MeV per nucleon (Cucinotta, Townsend, and Wilson). The cross section for triton production is (Cucinotta, Townsend, and Wilson):

Table 2.1: Threshold Energies for Alpha-Hydrogen Fragmentation Channels (Cucinotta, Townsend, and Wilson)

Fragmentation Channel	Threshold, MeV
${}^4\text{He} + \text{p} \rightarrow {}^2\text{H} + {}^3\text{He}$	22.94
${}^4\text{He} + \text{p} \rightarrow \text{p} + \text{p} + {}^3\text{H}$	24.77
${}^4\text{He} + \text{p} \rightarrow \text{p} + \text{n} + {}^3\text{He}$	25.72
${}^4\text{He} + \text{p} \rightarrow \text{p} + {}^2\text{H} + {}^2\text{H}$	29.81
${}^4\text{He} + \text{p} \rightarrow \text{p} + \text{p} + \text{n} + {}^2\text{H}$	32.59
${}^4\text{He} + \text{p} \rightarrow \text{p} + \text{p} + \text{p} + \text{n} + \text{n}$	35.37

$$\sigma_t^{Cucinotta} = 15.5 \left[\frac{2}{1 + e^{(T_{th}-T)/7}} - 1 \right] \left(1 - \frac{0.45}{1 + 7e^{-T/55}} \right)^3 \times \left[1 + 1.8 \sqrt{\frac{T}{550}} \right] \left(e^{(750-T)/4500} \right). \quad (2.29)$$

Lastly, the cross section for deuteron production is (Cucinotta, Townsend, and Wilson):

$$\sigma_d^{Cucinotta} = 17 \left[\frac{2}{1 + e^{(T_{th}-T)/12}} - 1 \right] \left(1 + \frac{\frac{0.21T}{145} - 0.21}{1 + e^{(145-T)/6}} \right) \left(e^{-T/3000} \right). \quad (2.30)$$

Another possible reaction channel is referred to as the pickup channel by Cucinotta, Townsend, and Wilson. This channel is essentially a coalescence channel and occurs when a neutron is removed from the alpha, which coalesces with the target proton. The cross section for the pickup channel is (Cucinotta, Townsend, and Wilson):

$$\sigma_{pickup}^{Cucinotta} = 48 e^{-(T-T_{th})^{1.7/1350}}. \quad (2.31)$$

Table 2.1 lists the threshold energies for each of the possible alpha fragmentation channels. In order to apply this model to any target, not just hydrogen targets, multiply

$\sigma_{pickup}^{Cucinotta}$ by $A_T^{1/3}$, $\sigma_{He-3}^{Cucinotta}$ by $A_T^{0.31}$, $\sigma_t^{Cucinotta}$ by $A_T^{0.31}$, and $\sigma_d^{Cucinotta}$ by $A_T^{0.42}$.

Helium-3 and Triton Fragmentation

Currently no models for helium-3 and triton fragmentation have been found in the open literature. However, in the code HZETRN there exists an undocumented model for helium-3 and triton break up in the subroutine LIFRAG. This subroutine also contains

the model described above for alpha fragmentation. This model seems very crude at first glance, but considering that there are only two possible fragmentation channels for each ion the actual fragmentation process itself is not very complex. The possible fragmentation channels for each ion are listed below in Table 2.2. The model states that the deuteron production cross section for tritons and helium-3 is 35 percent of the total reaction cross section (Wilson et. al. 1995). Therefore, the triton fragmentation model is (Wilson et. al. 1995):

$$\sigma_{nd} = 0.35 * \sigma_{reaction} \text{ and } \sigma_{pnn} = \sigma_{reaction} - \sigma_{nd} , \quad (2.32)$$

and the helium-3 fragmentation model is (Wilson et. al. 1995):

$$\sigma_{pd} = 0.35 * \sigma_{reaction} \text{ and } \sigma_{ppn} = \sigma_{reaction} - \sigma_{pd} . \quad (2.33)$$

Fragment Kinetic Energy Distributions

In order to choose the kinetic energies of fragments resulting from nucleus-nucleus collisions, a microscopic model for the estimation of energy degradation in nucleus-nucleus collisions developed at the Naval Research Laboratory by Tsao and collaborators is used. This model assumes that the kinetic energy distributions of fragmentation/spallation products in the projectile rest frame are Gaussian distributed, as is suggested by experimental data (Tsao et. al.). The variance of this Gaussian distribution has a parabolic dependence on the fragment mass (Tsao et. al.). The average kinetic energy of a fragment resulting from a nucleus-nucleus collision is (Tsao et. al.):

$$\langle KE \rangle = KE - \langle dKE \rangle = KE - (E_A - E_{\Delta A} - M_f) , \quad (2.34)$$

Table 2.2: Triton and Helium-3 Fragmentation Channels

Triton	Helium-3
${}^3\text{H} + \text{X} \rightarrow \text{X} + \text{p} + \text{n} + \text{n}$	${}^3\text{He} + \text{X} \rightarrow \text{X} + \text{p} + \text{p} + \text{n}$
${}^3\text{H} + \text{X} \rightarrow \text{X} + \text{n} + {}^2\text{H}$	${}^3\text{He} + \text{X} \rightarrow \text{X} + \text{p} + {}^2\text{H}$

where E_A is the total energy of the prefragment, $E_{\Delta A}$ is the total energy of the particles ablated by the prefragment, and M_f is the rest mass energy of the final fragment. The variance of the kinetic energy distribution is (Tsao et. al.):

$$\sigma_{dKE}^2 = \frac{9T_{eff}^2 \Delta A}{A_P} \left[\sqrt{\frac{2\langle dKE \rangle}{3T_{eff}}} + 1 \right]^2, \quad (2.35)$$

where T_{eff} is the effective reaction temperature in the collision center of mass:

$$T_{eff} = \frac{2}{3} q \sqrt{\Lambda}. \quad (2.36)$$

The Lorentz parameter, Λ , is:

$$\Lambda = \frac{\beta_{cm}}{\beta_0 \sqrt{\gamma_0}}, \quad (2.37)$$

where

$$\lambda_0 = \frac{1}{\sqrt{1 - \beta_0^2}}, \quad (2.38)$$

β_{cm} is the center of mass velocity, β_0 is the velocity of the prefragment rest frame, and q is the excitation energy per nucleon in the center of mass frame. More detailed information on how to calculate E_A , $E_{\Delta A}$, and q is provided in Appendix A-2.

III. NUCLEUS-NUCLEUS EVENT GENERATOR

Now that the theories of several independent nuclear models have been discussed in Chapter II a discussion of how they will work together to form a nucleus-nucleus event generator is needed. Included in this discussion are some additional approximations and physics concepts that help to complete the picture that the nuclear models in Chapter II began to describe.

Total and Total Reaction Cross Sections

The total cross section is not calculated directly from the optical model developed by Townsend and collaborators. The agreement of the total and total reaction cross sections as compared with experiment at energies around 2 GeV/nucleon is within about 3 percent (Townsend, Wilson, and Bidasaria, 1983A). For lower energies around 25 MeV/nucleon the agreement is on the order of 20 percent (Townsend, Wilson, and Bidasaria, 1983A). The error in the ratio of the total cross section to total reaction cross section is smaller than the error for the total cross section alone. Therefore, the ratio of the total cross section to total reaction cross section using the optical model is calculated using data that is given in the referenced paper:

$$R = \frac{\sigma_{tot}^{optical}}{\sigma_R^{optical}} . \quad (3.1)$$

Then to actually calculate the total cross section, the total reaction cross section from Tripathi and collaborators' parameterization of total reaction cross sections is multiplied by the ratio of the optical model total cross section to total reaction cross section:

$$\sigma_{tot} = R\sigma_R^{Tripathi}. \quad (3.2)$$

Using the given data to calculate the ratio in equation (3.1) restricts the available cross sections. Projectiles must have a charge less than 27, targets must have a charge less than 83, and kinetic energies must be between 25 and 22500 MeV per nucleon. No significant errors are expected for ratios obtained by interpolating between the target mass numbers or projectile mass numbers of nuclei given in Townsend and collaborator's paper. Tripathi and collaborators' parameterization of total reaction cross sections is a more accurate model with smaller error at low energies than the total reaction cross section model developed by Townsend and collaborators. Most importantly, Tripathi and collaborators' model has better agreement with experiment than Townsend and collaborator's total reaction cross section model for all energies. The total reaction cross section that was calculated from Tripathi and collaborators' parameterization, $\sigma_R^{Tripathi}$, will be reported as the total reaction cross section in this work. Tripathi's total reaction cross section has no restriction on the projectile target pair, but kinetic energies must be greater than or equal to 1 MeV per nucleon.

As an example, the total and total reaction cross sections for ^{12}C colliding with ^{12}C is plotted in Figure 3.1 as a function of projectile kinetic energy. This same colliding system will be used throughout the rest of this dissertation in order to provide examples

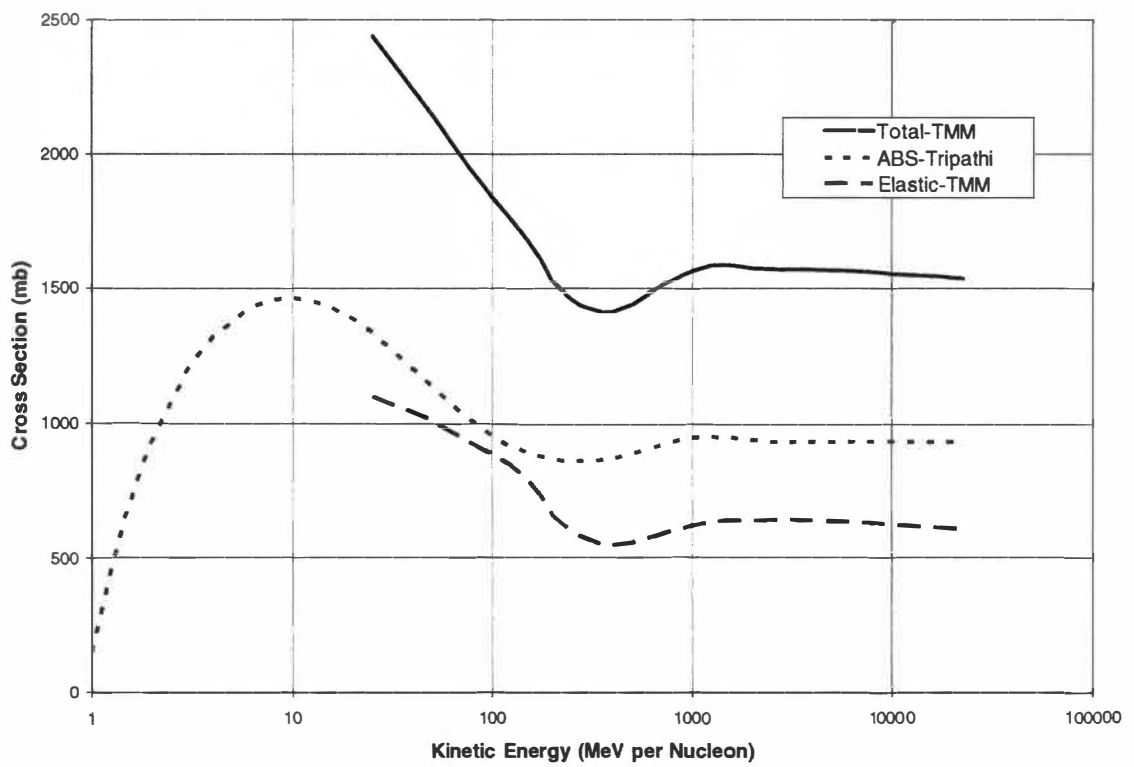


Figure 3.1: Total, Total Reaction, and Elastic Scattering Cross Sections for ^{12}C on ^{12}C

of other nuclear models as well. The total cross section in Figure 3.1 cuts off at 25 and 22500 MeV per nucleon because of the restriction imposed by the referenced data. The total reaction cross section cuts off at 1 MeV per nucleon due to the restriction of the nuclear model. However, the total reaction cross section can be calculated above 22500 MeV per nucleon. Below 25 MeV per nucleon the event generator uses the cross section value at 25 MeV per nucleon, and does not allow any fragmentation below 25 MeV per nucleon. While this may be a poor approximation of the cross section ions below 25 MeV per nucleon have a very small range and do not travel far. Above 22500 MeV per nucleon the event generator uses the cross section value at 22500 MeV per nucleon. Cross sections above about 3000 MeV per nucleon are fairly constant, so this is not a bad approximation.

Elastic Scattering Cross Section

The elastic scattering cross section is the difference between the total cross section and the total reaction cross section:

$$\sigma_{elastic} = \sigma_{tot} - \sigma_R^{Tripathi} . \quad (3.3)$$

Figure 3.1 also includes the elastic scattering cross section for ^{12}C on ^{12}C . In the event that an elastic scattering interaction occurs, particle kinematics is used to determine the new energy and direction of travel of the projectile and target. This simply involves applying conservation of energy and momentum before and after the collision:

$$\begin{aligned}
E_p + E_t &= E'_p + E'_t \\
P_p &= P'_p \cos \theta_p^z + P'_t \cos \theta_t^z + P'_p \cos \theta_p^x + P'_t \cos \theta_t^x + P'_p \cos \theta_p^y + P'_t \cos \theta_t^y,
\end{aligned} \tag{3.4}$$

where E is the total energy of the project or target before the collision, E' is the total energy of the projectile or target after the collision, P is the magnitude of the momentum vector for the projectile or target before the collision, P' is the magnitude of the momentum vector for the projectile or target after the collision, and θ is the angle for the projectile or target between the new direction of travel and the designated direction (x, y, or z). The resulting total energy of the projectile in the laboratory frame after the collision is (Byckling and Kajantie):

$$E'_p = \frac{(E_p + m_t) \{m_t E_p + m_p^2\} + P_p \cos \theta_p^z \sqrt{\{m_t E_p\}^2 - m_p^2 m_t^2 - m_p^2 P_p^2 \sin^2 \theta_p^z}}{(E_p + m_t)^2 - P_p^2 \cos^2 \theta_p^z} \tag{3.5}$$

With equation (3.5) and the energy equation in (3.4) the resulting total energy of the target in the laboratory frame can be calculated. To find the scattering angles the Fraunhofer approximation, which is a semiclassical approach, is applied. It states that the scattering angle of the projectile in the center of mass frame is approximated by the following distribution (Fraunfelder and Henley):

$$\frac{d\sigma}{d\Omega} = (kR_0^2)^2 \left(\frac{J_1(kR_0\theta)}{kR_0\theta} \right)^2, \tag{3.6}$$

where θ is the scattering angle, R_0 is the radius of the target, k is the wave number of the projectile, and J_1 is the first order Bessel function of the first kind. Figure 3.2 shows the differential elastic scattering cross section of ^{12}C on ^{12}C in the center of mass frame with projectile kinetic energies of 1000 and 25 MeV per nucleon as approximated by the

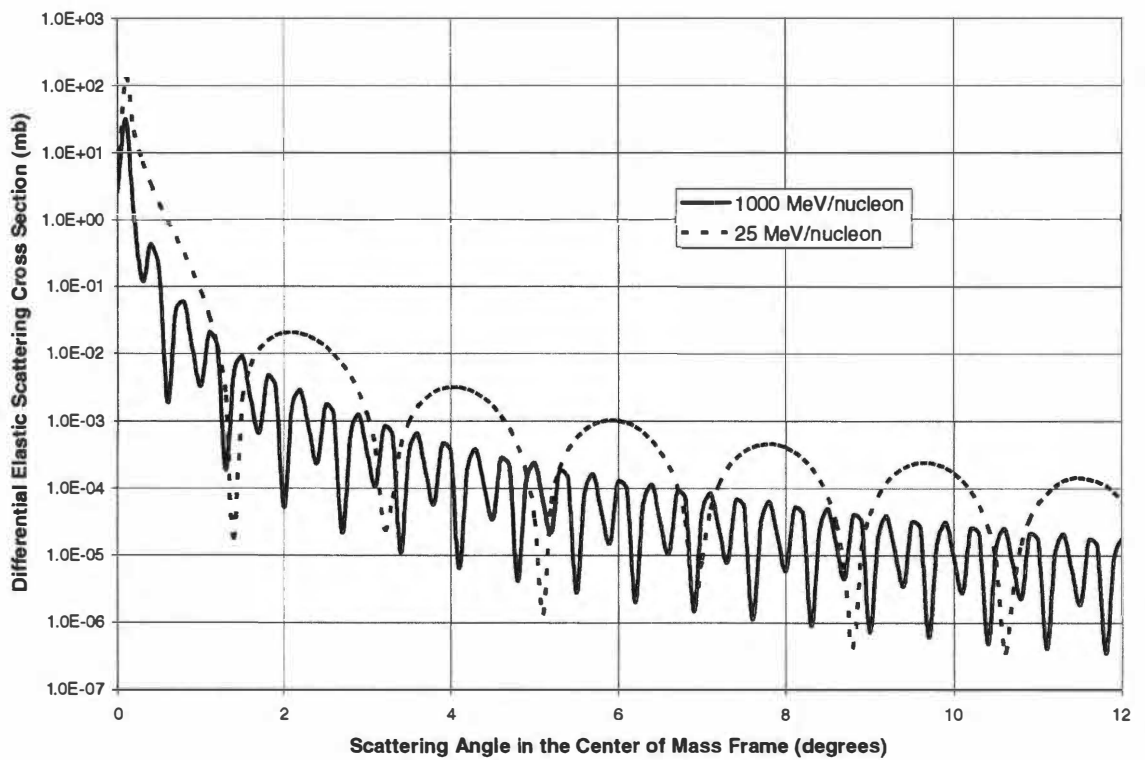


Figure 3.2: Differential Elastic Scattering Cross Section for ^{12}C on ^{12}C at 25 and 1000 MeV per Nucleon

Fraunhofer approximation. Sampling the distribution in equation (3.6) allows one to pick θ_p^{z*} , which is the scattering angle between the scattered projectile and the original direction of travel in the center of mass frame. The angle between the scattered target and the original projectile direction of travel in the center of mass frame is $\theta_t^{z*} = \pi - \theta_p^{z*}$. In order to transform these center of mass scattering angles to the laboratory frame use the following relationships (Byckling and Kajantie):

$$\begin{aligned}\tan \theta_p^z &= \frac{\sin \theta_p^{z*}}{\gamma \left(\cos \theta_p^{z*} + \frac{\beta^{cm}}{\beta_p^{cm*}} \right)}, \\ \tan \theta_t^z &= \frac{\sin \theta_p^{z*}}{\gamma \left(-\cos \theta_p^{z*} + \frac{\beta^{cm}}{\beta_t^{cm*}} \right)}\end{aligned}\quad (3.7)$$

where β^{cm} ($\beta = v/c$) is the relativistic velocity of the center of mass frame in the laboratory frame, β_p^{cm*} is the relativistic velocity of the projectile after the collision in the center of mass frame, β_t^{cm*} is the relativistic velocity of the target after the collision in the center of mass frame, and $\gamma = \left[1 - (\beta^{cm})^2 \right]^{-0.5}$. After the polar (z direction) scattering angle is chosen the remaining azimuthal scattering angles (between the x and y directions) for the target and projectile can be randomly sampled between 0-degrees and 360-degrees because elastic scattering is isotropic with respect to those angles.

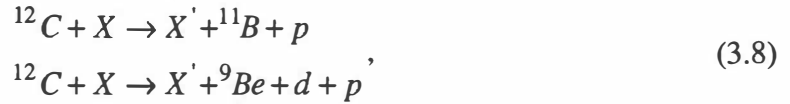
Double Differential Fragmentation/Spallation Production Cross Sections

Unfortunately, there is no single nuclear model currently available that is capable of accurately predicting double differential cross sections for the production of all secondaries from nuclear collisions at all of the energies of interest within a reasonable period of time (hours to days). Neither is there sufficient experimental measurements of these double differential cross sections to use in database development for space radiation shielding and transport studies. Therefore, several nuclear models must be used in conjunction to predict double differential production cross sections for nucleus-nucleus collisions.

Heavy Ion ($Z > 2$) Production Cross Sections

NUCFRG2 accurately accounts for the yields of all light ion and heavy ion fragments produced by a nucleus-nucleus collision, with a projectile charge number greater than 2. Given a nucleus-nucleus pair and beam energy, NUCFRG2 calculates the cross sections for each possible fragment/spallation product. However, in its original form the cross sections that NUCFRG2 provides are actually the probability of that fragment/spallation product being produced times the average multiplicity. This is adequate for deterministic codes, but for a Monte Carlo algorithm this probability and the multiplicity need to be separated. In reality this is only a problem for the light ion products because the average

multiplicity of the heavy ions in NUCFRG2 is one. In order to clearly explain this problem with the average multiplicity let's consider the following reactions:



where X is the target and X' is all the target fragments. Assuming the first reaction listed above produces ${}^{11}\text{B}$ with a cross section of 10 mb, then the proton produced in that collision also has a production cross section of 10 mb. If the second reaction has a cross section for producing ${}^9\text{Be}$ of 5 mb, then the deuteron and proton also have a 5 mb production cross section. NUCFRG2 keeps track of all of these production cross sections. At the end NUCFRG2 sums all the production cross sections for alphas, helium-3, tritons, deuterons, and protons and reports this sum for their respective production cross sections. So for our example in equation (3.8) ${}^{11}\text{B}$ has a cross section of 10 mb, ${}^9\text{Be}$ has a cross section of 5 mb, deuterons have a cross section of 5 mb, and protons have a cross section of 15 mb. As you can see the light ion cross sections contain more than just the cross section of that ion when it is the fragment. Therefore, for use in this nucleus-nucleus event generator, NUCFRG2 was modified. The modified version of NUCFRG2 is exactly the same as the original except for subroutine YIELDH. This is the subroutine where the original version added the cross sections for the light ions as the fragment with the cross sections for the light ions being ablated from the prefragment or abraded by the target. The modification simply involved commenting out the lines where these additional cross sections were added to the fragment cross section. Below Table 3.1 shows the production cross sections for ${}^{12}\text{C}$ on ${}^{12}\text{C}$ at 1 GeV per nucleon calculated

Table 3.1: Production Cross Sections for ^{12}C on ^{12}C at 1 GeV per Nucleon with Average Multiplicities for Light Ions (mb)

Charge	Mass	NF2	NF2-TMM	Charge	Mass	NF2	NF2-TMM
6	11	52.9027	52.9027	3	10	2.52E-03	2.52E-03
6	10	0.353754	0.353754	3	9	3.42E-02	3.42E-02
6	9	2.73E-03	2.73E-03	3	8	0.106091	0.106091
6	8	2.30E-06	2.30E-06	3	7	20.5311	20.5311
5	11	53.11982	53.11982	3	6	28.61594	28.61594
5	10	54.56862	54.56862	2	9	4.61E-06	4.61E-06
5	9	3.07356	3.07356	2	8	3.35E-05	3.35E-05
5	8	1.60E-02	1.60E-02	2	6	0.36744	0.36744
5	6	3.75E-06	3.75E-06	2	4	151.194	25.80074
4	10	3.299027	3.299027	2	3	11.72714	8.24591
4	9	13.15494	13.15494	1	6	3.33E-05	3.33E-05
4	8	3.452457	3.452457	1	3	23.45637	16.49329
4	7	18.95178	18.95178	1	2	61.88556	23.06178
4	6	7.85E-02	7.85E-02	1	1	4478.601	717.6099

by the original version of NUCFRG2 (labeled NF2). Also in Table 3.1 are the production cross sections for ^{12}C on ^{12}C at 1 GeV per nucleon calculated by the modified version of NUCFRG2 (labeled NF2-TMM). The differences between NUCFRG2 and the modified version of NUCFRG2 are in bold in Table 3.1.

One other correction that was necessary for NUCFRG2 dealt with neutron production. Looking at Table 3.1 one will notice that the neutron is not listed as a possible fragment. This is due to the nature of the NUCFRG2 model. It does not allow any neutron production in the fragmentation process, meaning that the remains of the fragment after ablation is never a neutron. Therefore, a rough estimate of the neutron production cross section, σ_{neutron} , can be attained by scaling the proton production cross section calculated by NUCFRG2, $\sigma_{\text{proton-nf2}}$:

$$\sigma_{\text{neutron}} = \frac{A_P - Z_P}{Z_P} \sigma_{\text{proton}}. \quad (3.9)$$

Continuing the example started in Table 3.1, neutron production cross section calculated using equation (3.9) would be 717.6099 mb.

Light Ion ($Z \leq 2$) Production Cross Sections

Deuteron Breakup

As was previously stated the deuteron breakup model is simply Tripathi's improved total reaction cross section model because there is only one possible reaction channel for a deuteron. Therefore, a Monte Carlo algorithm can be used to determine if the deuteron-nucleus interaction is elastic or inelastic. If the interaction is elastic then the process described previously about elastic scattering will determine the outcome of the reaction. If the interaction is inelastic then the reaction will produce a proton and a neutron. Figure 3.3 shows the deuteron on ^{12}C total reaction (or breakup) cross section as a function of projectile kinetic energy.

Alpha Fragmentation

Cucinotta and collaborators' model for alpha fragmentation/spallation will be used to determine the products of alpha-nucleus collisions. For alpha breakup the products of the reaction will actually be determined by choosing the entire reaction channel of the alpha breakup. The 5 possible fragmentation channels for alpha breakup were listed in Table 2.1. Figure 3.4 shows the fragmentation channel cross sections for an alpha on ^{12}C as a function of projectile kinetic energy. Figure 3.5 is the same as Figure 3.4 with the 2 proton 2 neutron channel removed to enable one to see the others more clearly.

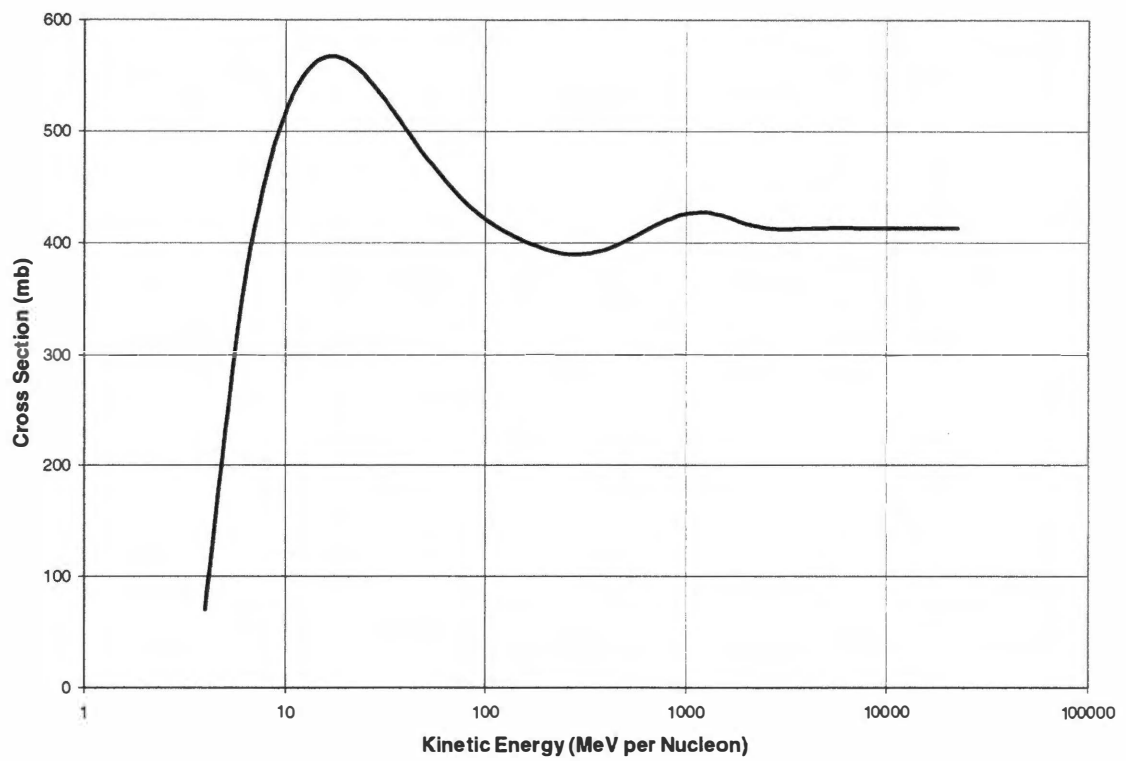


Figure 3.3: Deuteron on ^{12}C Total Reaction Cross Section

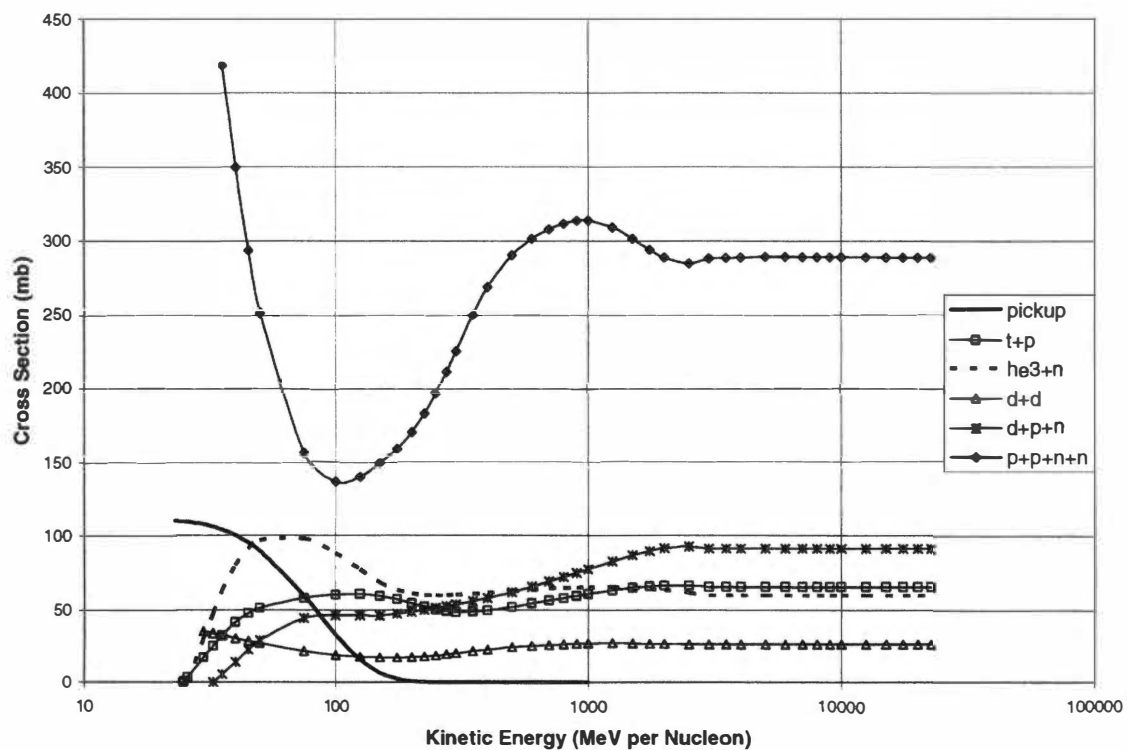


Figure 3.4: Alpha on ^{12}C Fragmentation Channel Cross Sections

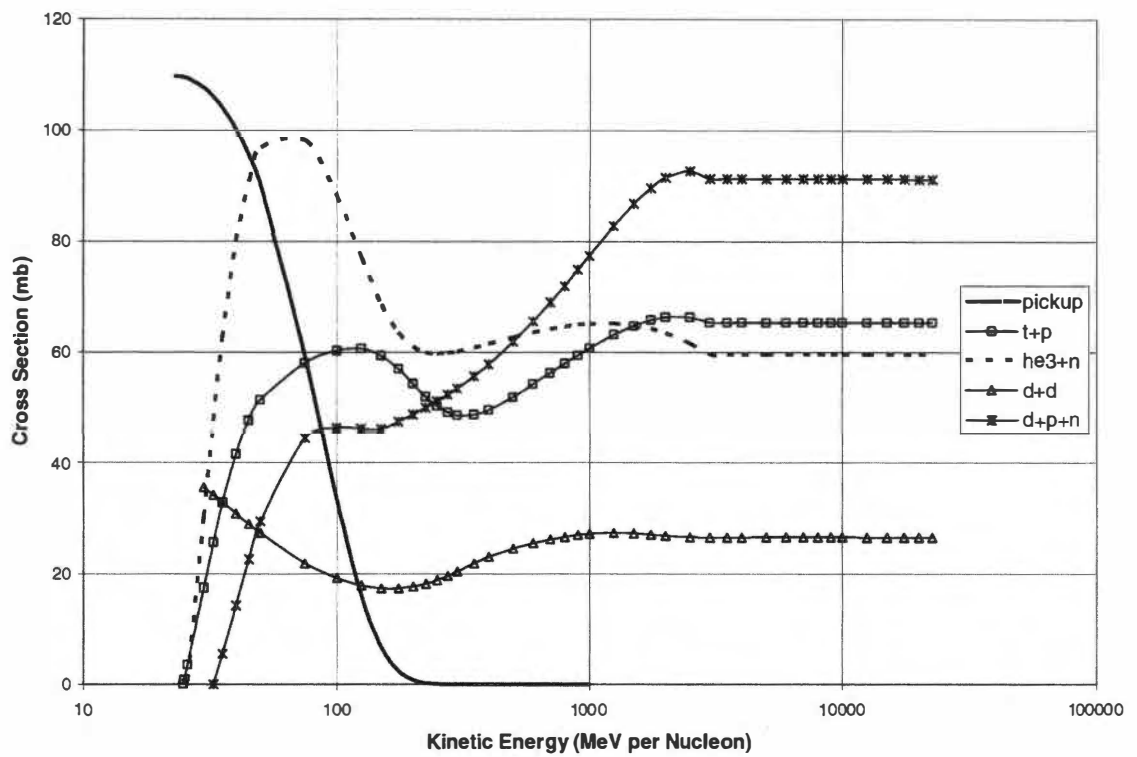


Figure 3.5: Alpha on ^{12}C Fragmentation Channel Cross Sections Excluding 2 p 2 n

Helium-3 and Triton Fragmentation

The remaining light ions are the triton and ^3He . The fragmentation models for each of these ions are very similar. Again, since there are only two fragmentation channels for each ion, the cross sections are used to pick the specific channels not just the individual fragments. This utilizes the property shown in equations (2.32) and (2.33) that the deuteron production cross section for triton and ^3He fragmentation is 35 percent of the total reaction cross section. Hence, if either ion undergoes an inelastic collision one merely samples whether a deuteron was produced or not. This determines which fragmentation channel has resulted from the collision. Figure 3.6 shows the fragmentation channel cross sections for a triton on ^{12}C as a function of projectile kinetic energy, and Figure 3.7 shows the fragmentation channel cross sections for a ^3He ion on ^{12}C as a function of projectile kinetic energy.

Fragment Kinetic Energy and Angular Distributions

Previously it was noted that the microscopic model for the estimation of energy degradation in nucleus-nucleus collisions assumes that the kinetic energy distributions of fragmentation/spallation products in the projectile rest frame are Gaussian distributed, as was suggested by experimental data (Tsao et. al.). This model calculates the mean and standard deviation of the corresponding fragment kinetic energy distribution. Using the mean and standard deviation, a Gaussian distribution is sampled in order to pick a kinetic

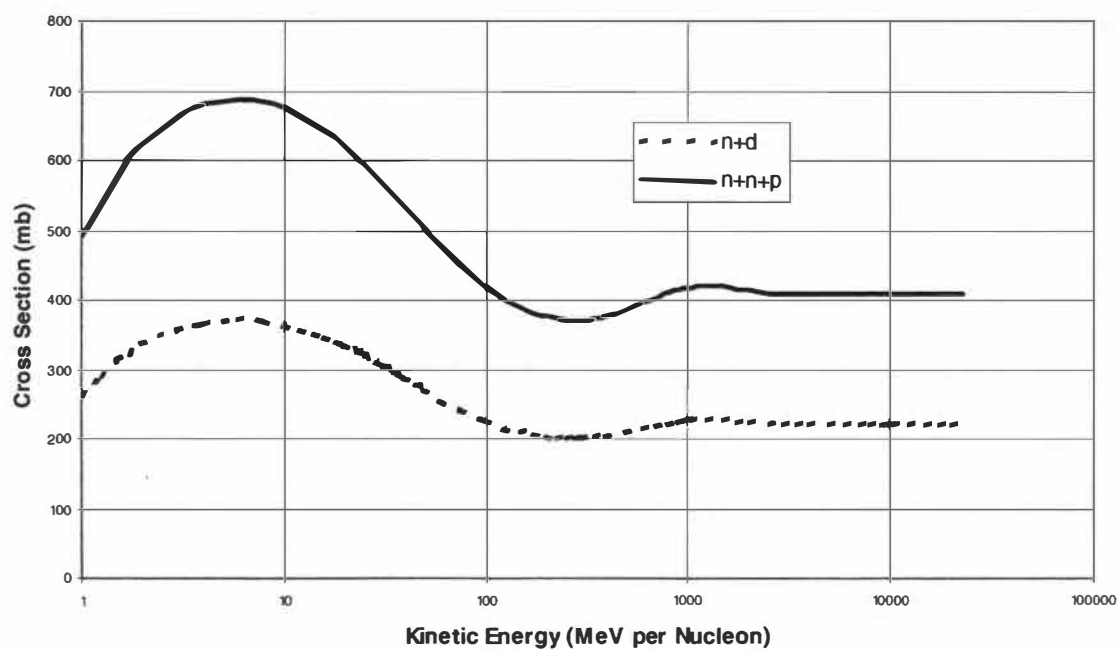


Figure 3.6: Triton on ^{12}C Fragmentation Channel Cross Sections

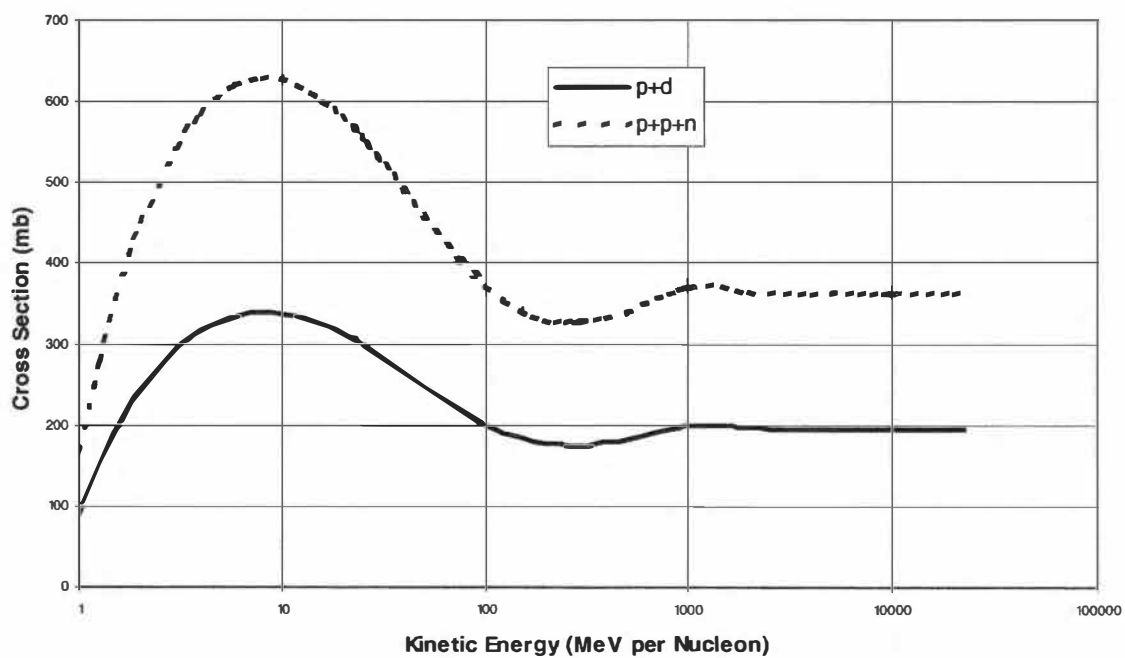


Figure 3.7: ^3He on ^{12}C Fragmentation Channel Cross Sections

energy for the fragment. To illustrate, once again consider the interaction of ^{12}C at 1 GeV per nucleon with ^{12}C . Below in Table 3.2 are two examples of possible fragmentation channels for this interaction. Also listed for both fragmentation channels are the mean and standard deviation of each particle's kinetic energy distribution as given by Tsao and collaborators' model. The mean and standard deviation in Table 3.2 are given in units of MeV per nucleon in the laboratory frame. Also previously discussed was the assumption that light fragments are coincident with a heavier fragment, and that both have the same mean kinetic energy per nucleon. This assumption essentially says that all particles are treated as the fragment, i.e. the remains of the prefragment after ablation, when the mean kinetic energy is calculated by this model. However, this model is being applied to not only the fragment but also light ions that are evaporated from the prefragment and nucleons that are abraded from the projectile. Therefore, this assumption is only used in the nucleus-nucleus event generator for heavy fragments. When the mean and standard deviation of the kinetic energy distribution is being calculated for an evaporated particle or an abraded nucleon this assumption is not used. This allows for a broader range of kinetic energies to be realized, which is more consistent with experimental measurements of light ions and nucleons. To illustrate the difference, Table 3.3 shows the same particles resulting from the same interactions as Table 3.2, however, the model by Tsao and collaborators' has now been modified. In Table 3.3 it is clear that the evaporated and abraded particles will have a broader range of kinetic energies than the evaporated and abraded particles in Table 3.2. The slight differences in the mean and standard deviations of the fragments are due to two other

Table 3.2: Example Means and Standard Deviations for Fragment Kinetic Energy

Distributions of ^{12}C at 1 GeV per nucleon on ^{12}C

$^{12}\text{C} + ^{12}\text{C} \rightarrow \text{X} + ^{11}\text{B} + \text{p}$				$^{12}\text{C} + ^{12}\text{C} \rightarrow \text{X} + ^7\text{Li} + ^3\text{He} + \text{p} + \text{n}$			
Charge	Mass	Mean	Standard Deviation	Charge	Mass	Mean	Standard Deviation
5*	11*	982.2	24.94	3*	7*	974.1	60.66
1	1	977.7	86.89	2	3	969.0	84.83
				1	1	977.7	86.89
				0	1	972.2	95.44
*Fragment, i.e. remains of prefragment after ablation (MeV per nucleon)							

Table 3.3: Example Means and Standard Deviations for Fragment Kinetic Energy

Distributions of ^{12}C at 1 GeV per nucleon on ^{12}C – Modified Model

$^{12}\text{C} + ^{12}\text{C} \rightarrow \text{X} + ^{11}\text{B} + \text{p}$				$^{12}\text{C} + ^{12}\text{C} \rightarrow \text{X} + ^7\text{Li} + ^3\text{He} + \text{p} + \text{n}$			
Charge	Mass	Mean	Standard Deviation	Charge	Mass	Mean	Standard Deviation
5*	11*	982.2	25.64	3*	7*	974.1	62.87
1	1	795.5	179.3	2	3	934.5	109.7
				1	1	795.5	179.3
				0	1	794.6	179.6
*Fragment, i.e. remains of prefragment after ablation (MeV per nucleon)							

changes made in the model. First, the rest mass energies of all particles in the original version of the model were calculated using a liquid drop model. Now the rest mass energies are calculated using mass excess data (Audi and Wapstra) and the relationship between a nucleus's mass excess, Δ , and rest mass energy:

$$M = \Delta + (931.494013 * A) - (Z * M_{e^-}), \quad (3.10)$$

where A is the nucleus mass number, Z is the nucleus charge number, and M_{e^-} is the electron rest mass energy. Second, the convergence criterion on equation (A.36) was originally set to 0.01, but now has been changed to 0.0001. This change in the convergence affects the value of the excitation energy per nucleon in the center of mass frame, q .

Another important parameter in the nucleus-nucleus event generator's kinetic energy model is the Fermi energy of a particle emitted by a projectile. This is the kinetic energy the individual neutrons and protons have while internally confined in the nucleus according to the Fermi Gas Model. To calculate the Fermi energy first calculate the Fermi momentum (Rith, et. al., p. 242):

$$\begin{aligned} P_F^{proton} &= \sqrt[3]{\frac{9\pi^2 \hbar^3 Z_p}{4\pi R^3}} \\ P_F^{neutron} &= \sqrt[3]{\frac{9\pi^2 \hbar^3 (A_p - Z_p)}{4\pi R^3}} \end{aligned}, \quad (3.11)$$

where Z_p is the charge number of the projectile, A_p is the mass number of the projectile, and R is the radius of the projectile. Now the Fermi energy is found by (Rith, et. al., p. 242):

$$\begin{aligned} E_F^{proton} &= \frac{(P_F^{proton})^2}{2M_p} \\ E_F^{neutron} &= \frac{(P_F^{neutron})^2}{2M_n} \end{aligned} \quad (3.12)$$

where M is the rest mass energy of the proton or neutron. The Fermi energy of a particle emitted by the projectile is:

$$E_F^{fragment} = \frac{Z_f E_F^{proton} + (A_f - Z_f) E_F^{neutron}}{A_f}, \quad (3.13)$$

where Z_f is the charge number of the emitted particle and A_f is the mass number of the emitted particle. Since this kinetic energy and momentum are the kinetic energy and momentum inside the nucleus it is assumed that the values calculated in equations (3.11), (3.12), and (3.13) are in the projectile rest frame. What is significant about the Fermi energy is that it is an estimate of the maximum kinetic energy gain or minimum kinetic energy loss a particle may have upon being emitted from the projectile in the projectile rest frame. Therefore, it is used to limit the standard deviation of the fragment (the remains of the prefragment) by:

$$\begin{aligned} \langle KE^{fragment} \rangle - E_F^{fragment} &\leq \langle KE^{fragment} \rangle - 3\sigma^{fragment} \\ \langle KE^{fragment} \rangle + E_F^{fragment} &\geq \langle KE^{fragment} \rangle + 3\sigma^{fragment} \end{aligned} \quad (3.14)$$

where $\langle KE^{fragment} \rangle$ and $\sigma^{fragment}$ are the mean and standard deviation reported by the modified version of Tsao and collaborators' model. In the case of evaporated and abraded particles the limit set in equation (3.14) becomes:

$$\langle KE^{fragment} \rangle + E_F^{fragment} \geq \langle KE^{fragment} \rangle + 3\sigma^{fragment}. \quad (3.15)$$

The lower limit in equation (3.14) is not enforced for evaporated and abraded particles in an attempt to model the broad energy range of these particles, which is lower than what the Fermi energy will allow. This is important because meson production is not currently modeled by this nucleus-nucleus event generator. Mesons, like the pion, can be produced in nucleus-nucleus collisions. Single pion production in nucleon-nucleon collisions has a threshold energy of about 290 MeV, while double pion production in nucleon-nucleon collisions has a threshold energy of about 600 MeV (Krane, p. 670). Pions can be charged, and therefore undergo continuous slowing down like all other charged particles. However, these pions can subsequently produce nucleons via interactions or decay, and these nucleons can have kinetic energies outside the lower limit set by the Fermi energy in equation (3.14). This is somewhat analogous to the phenomenon of delayed neutrons seen in nuclear fission reactions. Therefore, equation (3.15) is how the Fermi energy is used to limit the modified version of Tsao and collaborators' model for evaporated and abraded particles.

Finally, the angular distribution of particles produced in nucleus-nucleus interactions must be considered. This event generator does not use a specific nuclear model for selecting scattering angles during particle production. Instead it applies a few

systematics of momentum distributions observed during experiments by Morrissey (1989). First, Morrissey stated that longitudinal momentum distributions of projectile-like particles are roughly isotropic in a rest frame moving with nearly the beam velocity. Therefore, the event generator samples scattering angles of particles emitted by the projectile isotropically in the projectile rest frame. Second, Morrissey stated that target-like particles' momentum distributions are essentially isotropic in a frame nearly at rest. Therefore, the event generator samples scattering angles of particles emitted by the target isotropically in the target rest frame, which is equivalent to the laboratory frame.

Projectile and Target Role Reversal

To this point this discussion of the nucleus-nucleus event generator has centered on the projectile. That is because after the event generator chooses the projectile fragments and their energies and angles the role of projectile and target are reversed. Then with the actual target in the role of the projectile this same process is repeated to choose the target fragments and their energies and directions. The target, now in the role of the projectile, maintains the same kinetic energy per nucleon as the projectile. Essentially, the process of determining the results of target fragmentation is the same as determining the results of projectile fragmentation. However, one difference does exist. After the kinetic energies of the projectile fragments have been chosen they are transformed from the projectile rest frame back to the laboratory frame. After the kinetic energy of the target fragments have been chosen they are not transformed from the target rest frame to the laboratory frame

rather they are transformed from the target rest frame to the frame of the recoiling target. This models the fact that the projectile does transfer some kinetic energy to the target. Otherwise the kinetic energy of the target fragments would all nearly be zero because the target rest frame and laboratory frame are equivalent. The kinetic energy of the recoiling target, KE_T' , is defined as:

$$KE_T' = E_P + E_T - \sum_{i=1}^n E_{P_f}^i - \sum_{j=1}^m M_{T_f}^j, \quad (3.16)$$

where E_P and E_T is the total energy of the target and projectile before the collision, $E_{P_f}^i$ is the total energy of the i^{th} particle emitted by the projectile, with a total of n particles emitted by the projectile, and $M_{T_f}^j$ is the rest mass energy of the j^{th} particle emitted by the target, with a total of m particles emitted by the target.

IV. HETC-HEDS

The nucleus-nucleus event generator that was described in Chapter III has been added as a module to the Monte Carlo radiation transport code HETC to create HETC-HEDS. This chapter contains a brief description of HETC's capabilities, and then gives details about the event generator's coding structure and what was done to make it a module in HETC. An HETC-HEDS user's manual is located in Appendix B, and the actual coding of the nucleus-nucleus event generator is located in Plate 1 (the CD-ROM attached to this dissertation).

HETC

HETC simulates the projectile interactions with target nuclei by using Monte Carlo techniques to compute the trajectories of the primary particle and the secondary particles produced in nuclear collisions. The particles considered by HETC (protons, neutrons, $\pi^\pm$, and $\mu^\pm$) may be arbitrarily distributed in angle, energy, and space. Neutrons produced below a given cutoff, usually 20 MeV, and photons produced in the interactions or from deexcitation gammas are not transported. Instead, their position, energy, and angular information are stored for transport by codes such as MORSE and EGS, as part of the CALOR package (Gabriel et. al.), MCNP (Brown), or MCNPX. The methods used to describe the physical interactions of the projectile and target are described next.

The energy loss of protons, charged pions, and muons due to the excitation and ionization of atomic electrons is treated using the well-established Bethe-Bloch stopping power formula (equation 1.12) based on the continuous slowing-down approximation (Rossi). Range-energy tables for each material in the system are computed for protons. These same tables are used for charged pions and muons by making use of scaling relations (Coleman).

Multiple Coulomb scattering of primary particles is treated using Fermi's joint distribution function for angular and lateral spread and Rutherford's single-scattering cross-section formula (Rossi). HETC is presently programmed to allow multiple Coulomb scattering only for the primary charged particles.

Charged-pion decay in flight is taken into account using the known pion lifetime. The energy and angular distribution of the muon produced in the decay is obtained by assuming that the pion decay is isotropic in the rest frame of the pion. The distribution is then transformed from the pion rest frame into the laboratory system. A π^+ , which comes to rest, is assumed to decay immediately into a μ^+ and a neutrino, and the energy and angular distribution of the muon is obtained in the same manner as discussed above for pion decay. A π^- , which comes to rest, may either decay or be captured by a nucleus. If captured the energy and angular distributions of the particles produced are obtained using the intranuclear-cascade-evaporation model described below. The neutral pion is very unstable and may be assumed to decay into two photons at its point of origin.

Accordingly, HETC does not transport neutral pions, although their production is included as part of the output.

Muons are unstable and decay into electrons or positrons and neutrinos. Muon decay in flight is taken into account using the known muon lifetime, and muons that come to rest are assumed to decay immediately. No information for the electrons, positrons, or neutrinos from muon decay is calculated.

Elastic collisions of protons and pions with all nuclei other than hydrogen are neglected at all energies. Elastic collisions by neutrons with nuclei other than hydrogen at energies above the neutron cutoff energy (usually 20 MeV) are optional in HETC, and if the option is chosen, require the input of elastic scattering cross section data. Elastic collisions of protons, neutrons and charged pions with hydrogen nuclei are treated using experimental data and/or parametric fits to experimental data (Gabriel, Santoro, and Barish; Ranft and Borek).

Pion production is based on the isobar model of Sternheimer and Lindenbaum. The particle cross sections are based on experimental data and/or models. Only single and double pion production in nucleon-hydrogen collisions and single pion production in pion-nucleon collisions are accounted for. This model is used for energies up to 3.5 GeV for neutrons and protons, and up to 2.5 GeV for charged pions. Nonelastic nucleon collisions and charged pion collisions with hydrogen nuclei at energies above 3.5 GeV

and 2.5 GeV are treated by using the calculational methods of Gabriel, Santoro, and Barish and Ranft and Borek, respectively.

The intranuclear-cascade evaporation concept of particle-nucleus interactions, as implemented by Bertini, is used to determine the effect of particle-nucleus collisions below 3.5 GeV for nucleons and 2.5 GeV for charged pions. This model has been used for a variety of calculations and has been shown to agree well with many experimental results in the energy range below 3 GeV. The types of particle collisions included in the calculation are elastic, inelastic, and charge exchange. Following the intranuclear-cascade, there is excitation energy left in the nucleus. This residual energy is treated using an evaporation model (Guthrie). The particles allowed during evaporation include protons, neutrons, deuterons, tritons, ^3He , and alphas.

An extrapolation model determines the energy, angle, and multiplicity of the products from inelastic nucleon-nucleus and pion-nucleus collisions at higher energies (≥ 3 GeV and ≤ 15 GeV) (Gabriel, Alsmiller, and Guthrie). This extrapolation method employs the particle-production data obtained from an intranuclear-cascade calculation for intermediate-energy (~ 3 GeV) nucleon-nucleus and pion-nucleus collisions, together with energy, angle, and multiplicity scaling relations that are consistent with the sparse experimental data available for high-energy collisions, to estimate the particle production for higher energy (≥ 3 GeV) collisions. This method applies to only those particles produced in the cascade phase of the collision; particle emission resulting from the

deexcitation of the residual nucleus is carried out by performing an evaporation calculation in the same manner as for nonscaled collisions.

HETC-HEDS

HETC-HEDS has all of the capabilities of HETC plus the event generator that was previously described for transport of projectiles with mass number greater than 1. One item that is not part of the nucleus-nucleus event generator, but is required for the transport of particles with mass number greater than 1, are range energy tables. These tables are needed to apply the continuous slowing down approximation to the charged projectiles, and they are calculated by scaling the proton values for the target media.

The nucleus-nucleus event generator described in Chapter III has been programmed using the FORTRAN 77 language. The event generator was developed on a PC using the HP/Compaq Visual FORTRAN Compiler. It has also been used on a SUN work station and SGI work station using the SUN and SGI FORTRAN compilers, respectively. HETC in its current state has only been used on an SGI work station, therefore, HETC-HEDS has only been run on an SGI work station. The event generator consists of 16 subroutines (including the main program) and 6 functions. These are all described below. A chart of the program structure is shown in Figure 4.1.

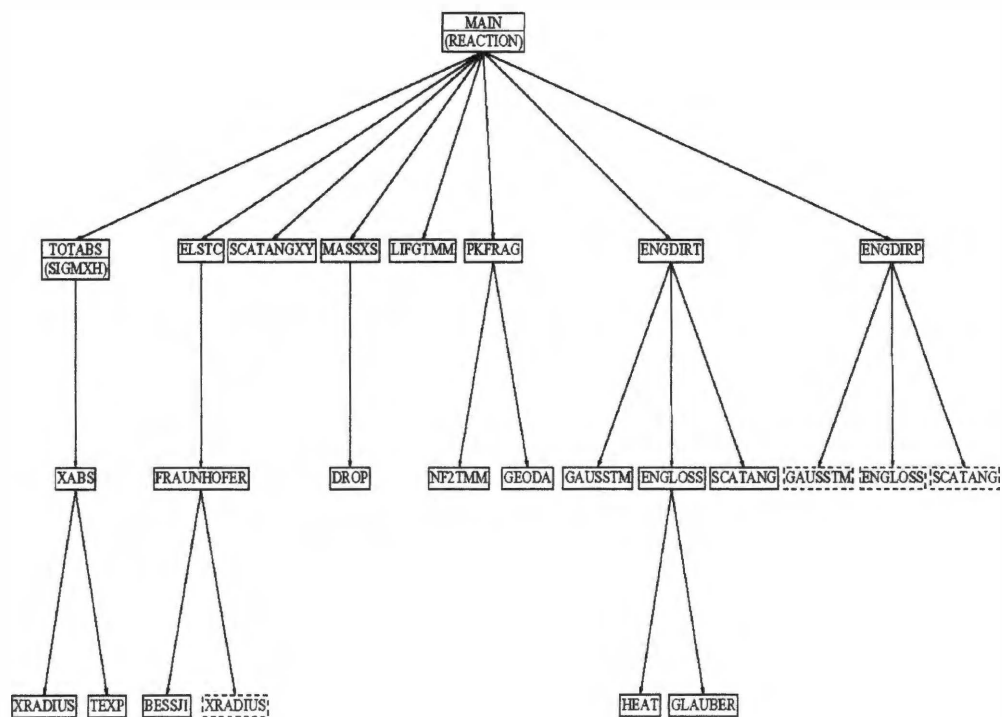


Figure 4.1: Nucleus-Nucleus Event Generator Program Structure

MAIN Program (REACTION)

The MAIN program is the driver of the nucleus-nucleus event generator. In the event generator MAIN begins by prompting the user for the required inputs of the problem:

- The charge and mass numbers of the projectile and target
- The kinetic energy of the projectile in MeV per nucleon in the laboratory frame
- What ablation method is to be used
- The number of histories to be simulated
- The name of the output file.

The event generator then calls subroutine TOTABS in order to calculate the total, total reaction, and elastic cross sections. Next the event generator begins to loop over the number of histories or number of interactions to be simulated. If it is determined that the interaction is an elastic collision subroutine ELSTC is called to determine the resulting projectile and target kinetic energies and scattering angles. It is assumed that the projectile is originally traveling in the Z direction. Next the subroutine SCATANGXY is called to calculate the direction cosines with respect to the X, Y, and Z directions. If it is determined that the interaction is an inelastic collision subroutine PKFRAG or LIFGTMM is called to determine the projectile fragments. Then the projectile and target are reversed and subroutine PKFRAG or LIFGTMM is called again to determine the target fragments. Next, MAIN loops over the projectile fragments and calls the subroutine ENGDIRP to determine the kinetic energies and direction cosines of each projectile fragment. Then MAIN loops over the target fragments and calls the subroutine

ENGDIRT to determine the kinetic energies and direction cosines of each target fragment. Finally, MAIN prints the results of each history in the output file.

The MAIN program of the event generator is the subroutine named REACTION in HETC-HEDS. The input needed for REACTION is passed via the subroutine call of REACTION. However, an additional parameter is provided which tells REACTION whether or not the current interaction is elastic or inelastic. With this information it is not necessary for REACTION to call TOTABS. The ablation method to be used is not passed as input to REACTION. Instead that is defined as a fixed parameter before the subroutine is compiled. In order to change the ablation method the subroutine must be changed and recompiled. The rest of REACTION works the same as MAIN, except that at the end of REACTION nothing is printed. Instead that information is passed back to the subroutine which called REACTION. The subroutine that calls REACTION is CASCADH.

Subroutine TOTABS (SIGMXH)

This subroutine is where the event generator calculates the ratio of the total cross section to the total reaction cross section using Townsend and collaborators' optical model (equation 3.1). Then Tripathi's total reaction cross section is calculated by calling the function XABS. Finally, the total and elastic cross sections are calculated (equations 3.2 and 3.3).

In HETC-HEDS this subroutine is named SIGMXH. SIGMXH works exactly the same as TOTABS, but SIGMXH is not called by REACTION. Instead, SIGMXH is called by CASCADH to determine if the interaction is elastic or inelastic and by GETFLTH to determine the location of the next interaction via the method of fictitious scattering (Cramer).

Function XABS

This is where Tripathi and collaborators' improved total reaction cross section is calculated (equation 2.13). XABS calls the functions XRADIUS and TEXP.

Function XRADIUS

This function calculates the radius of the given nucleus using experimental data compiled by De Vries, De Jager, and De Vries.

Function TEXP

TEXP simply calculates $\text{EXP}(x)$, but TEXP limits the size of x . This prevents CPU overflow or underflow. The input, x , is limited to the domain $-80 \leq x \leq 80$. If x is outside of this domain TEXP returns $\text{EXP}(-80)$ or $\text{EXP}(80)$ depending on which is closer to the actual value.

Function MASSXS

The function MASSXS calculates the rest mass energy of a given ion (equation 3.10). Mass excess data is taken from Audi and Wapstra. If no mass excess data is available a liquid drop model is used to calculate the rest mass energy, function DROP.

Function DROP

This function calculates the rest mass energy of a given ion using a liquid drop model.

Subroutine ELSTC

ELSTC calculates the kinetic energies and Z scattering angles of the projectile and target in an elastic collision (equations 3.4, 3.5, and 3.7). This subroutine calls subroutine FRAUNHOFER.

Subroutine FRAUNHOFER

The subroutine FRAUNHOFER samples the Z scattering angle for the projectile in an elastic collision (equation 3.6). FRAUNHOFER calls the functions XRADIUS and BESSJ1.

Function BESSJ1

This function calculates the value of the first order Bessel function of the first kind at the given point.

Subroutine SCATANGXY

Given the magnitude of a particle's momentum vector and Z scattering angle SCATANGXY calculates the X, Y, and Z direction cosines. In this process the X and Y scattering angles are sampled, which are chosen to conserve momentum.

Subroutine PKFRAG

PKFRAG determines the fragments of the projectile if the projectile has a charge number greater than 2. The fragment (the remains of the prefragment) is chosen from the cross sections calculated in the subroutine NF2TMM. If ablation method one or two is used the number of particles abraded and ablated are determined by calling the subroutine GEODA. Ablation method one ablates particles via NUCFRG2's methodology (equation A.31). Ablation method two samples the species of ablated particles where the probability of a particle being ablated is that particle's binding energy per nucleon. Finally, ablation method three assumes that all ablated particles are neutrons and protons. All abraded particles are assumed to be neutrons and protons.

Subroutine NF2TMM

This subroutine contains the modified version of NUCFRG2, which was discussed previously in Chapters II and III and also in Appendix A-1. The subroutine that was modified is YIELDH. Since NUCFRG2 is a well documented independent nuclear model in its own right I will not discuss its programming structure.

Subroutine GEODA

GEODA is a subroutine that is part of NUCFRG2, but is also used by the event generator independent of NUCFRG2 after the fragment (the remains of the prefragment) has been chosen. With the projectile and target mass and charge numbers and the fragment mass number GEODA calculates the number of nucleons abraded and ablated (Appendix A-1).

Subroutine LIFGTMM

Light ion ($Z \leq 2$) fragmentation, which is not modeled in PKFRAG, is modeled in LIFGTMM. If the projectile is an alpha particle the cross section for each fragmentation channel is calculated using equations 2.28, 2.29, 2.30, and 2.31. The cross section for each fragmentation channel of the triton is calculated using equation 2.32 and equation 2.33 if the projectile is a ^3He ion.

Subroutine ENDIRP

The subroutine ENDIRP calculates the kinetic energy and direction cosines for each projectile fragment. First it calls the subroutine ENGLOSS which returns the mean and standard deviation of the fragment kinetic energy distribution in the projectile rest frame. Then the subroutine GAUSSTM is called to sample a kinetic energy from the Gaussian kinetic energy distribution. Next a Z scattering angle is chosen by calling the subroutine SCATANG. Finally the subroutine SCATANGXY is called to calculate the X, Y, and Z direction cosines of the fragment.

Subroutine ENGLOSS

The microscopic model for the estimation of energy degradation in nucleus-nucleus collisions, which was described in Chapters II and III and Appendix A-2, is contained in this subroutine. The mean of the fragment kinetic energy distribution is calculated by equation 2.34 and the standard deviation by equation 2.35. ENGLOSS calls subroutines GLAUBER and HEAT.

Subroutine GLAUBER

This subroutine calculates the number of nucleons in the projectile spectator, target spectator, and participant for the model in ENGLOSS (equation A.32)

Subroutine HEAT

HEAT calculates the excitation energy per nucleon in the center of mass frame for the given nucleus-nucleus collision as needed by the model in ENGLOSS (equation A.36).

Subroutine GAUSSTM

The subroutine GAUSSTM, provided a mean and standard deviation, samples a Gaussian distribution.

Subroutine SCATANG

The kinetic energy that is sampled by GAUSSTM determines if the particle is going in the forwards or backwards direction in the projectile rest frame. However, SCATANG samples exactly what the scattering angle of the particle with respect to the Z axis is. SCATANG, like SCATANGXY, tries to conserve momentum.

Subroutine ENGDIRT

This subroutine is exactly like ENGDIRP, except that it calculates the kinetic energy and direction cosines for target fragments. The only difference between ENGDIRP and

ENGDIRT lies in what reference frames the Z scattering angle is chosen for projectile and target fragments. This difference was discussed in Chapter III.

V. EVENT GENERATOR & HETC-HEDS SAMPLE RESULTS

In order to better illustrate the capabilities of the newly created nucleus-nucleus event generator and HETC-HEDS several calculations have been performed. The calculations with the event generator are to show that its results can be used to reproduce some of the inputs provided by a few of the event generator's constituent models. Each of the HETC-HEDS calculations makes a direct comparison with an experiment whose results have been published in the open literature.

Sample Event Generator Results

First the event generator was run to calculate the fragmentation cross sections of ^{12}C at 1 GeV per nucleon on ^{12}C . This is an attempt to duplicate the results that were given by the modified version of NUCFRG2 previously listed in Table 3.1. The event generator simulated ten million histories that resulted in inelastic collisions. The fragments (i.e., the remains of the prefragment) were counted and the probability of producing those fragments was calculated. The probability of producing each fragment was multiplied by the sum of the production cross sections in Table 3.1 to calculate production cross sections using the event generator. This mean production cross section for each fragment and the standard deviation of the mean for each fragment are reported in Table 5.1. The values in Table 3.1 are also repeated in Table 5.1. A few cross sections in Table 5.1 were calculated as zero. Two (^{10}Li and ^9He) are zero because even though NUCFRG2

Table 5.1: Event Generator Calculated Production Cross Sections for ^{12}C on ^{12}C at 1 GeV
per Nucleon (mb) Compared to the Modified Version of NUCFRG2

Charge	Mass	NF2-TMM	Cross Section Calculated by Event Generator	Standard Deviation
6	11	52.9027	52.99084	0.095149
6	10	0.353754	0.353876	0.007894
6	9	2.73E-03	0.002818	0.000705
6	8	2.30E-06	0	
5	11	53.11982	53.15148	0.095288
5	10	54.56862	54.50833	0.096459
5	9	3.07356	3.086417	0.023296
5	8	1.60E-02	0.016558	0.001708
5	6	3.75E-06	0	
4	10	3.299027	3.297087	0.024077
4	9	13.15494	13.17514	0.047994
4	8	3.452457	3.420213	0.024521
4	7	18.95178	19.0015	0.057541
4	6	7.85E-02	0.070458	0.003523
3	10	2.52E-03	0	
3	9	3.42E-02	0.033291	0.002422
3	8	0.106091	0.107272	0.004347
3	7	20.5311	20.51141	0.059757
3	6	28.61594	28.7071	0.070528
2	9	4.61E-06	0	
2	8	3.35E-05	0.000176	0.000176
2	6	0.36744	0.382588	0.008208
2	4	25.80074	25.7151	0.066809
2	3	8.24591	8.215239	0.037952
1	6	3.33E-05	0	
1	3	16.49329	16.41445	0.05352
1	2	23.06178	23.01056	0.063248
1	1	717.6099	718.2144	0.273728
0	1	717.6099	717.0664	0.273659

calculates a cross section they physically are not possible. These ions have more neutrons than the projectile, so they are considered impossible to produce. The remaining ions with zero cross sections (^8C , ^6B , and ^6H) are not produced often enough to be sampled in ten million histories.

Next, using the same example of ^{12}C at 1 GeV per nucleon on ^{12}C , the mean and standard deviation of each fragments' kinetic energy distribution for the reaction channel whose fragment (i.e. remains of the prefragment) is ^7Li , discussed in Tables 3.2 and 3.3, were calculated. This is an attempt to reproduce the results listed in Table 3.3. First, one million samples of the ^7Li kinetic energy distribution were collected in bins and plotted against the Gaussian function with the sample mean and standard deviation. These million samples were taken independent of the other distributions, so conservation of energy was not required when taking these samples. This comparison is in Figure 5.1. Then one million samples of each fragments' kinetic energy distribution were taken, requiring energy to be conserved. The resulting mean kinetic energies and standard deviations (of the sample, not the mean) for each fragment are shown in Table 5.2. The values from Table 3.3 are also repeated in Table 5.2. The values in Table 5.2 are in units of MeV per nucleon in the laboratory frame.

The final calculation done with the event generator looked at the momentum of the fragments produced by the reaction channel discussed in Table 5.2. This is an attempt to look at momentum conservation for projectile fragments in the projectile rest frame. As a

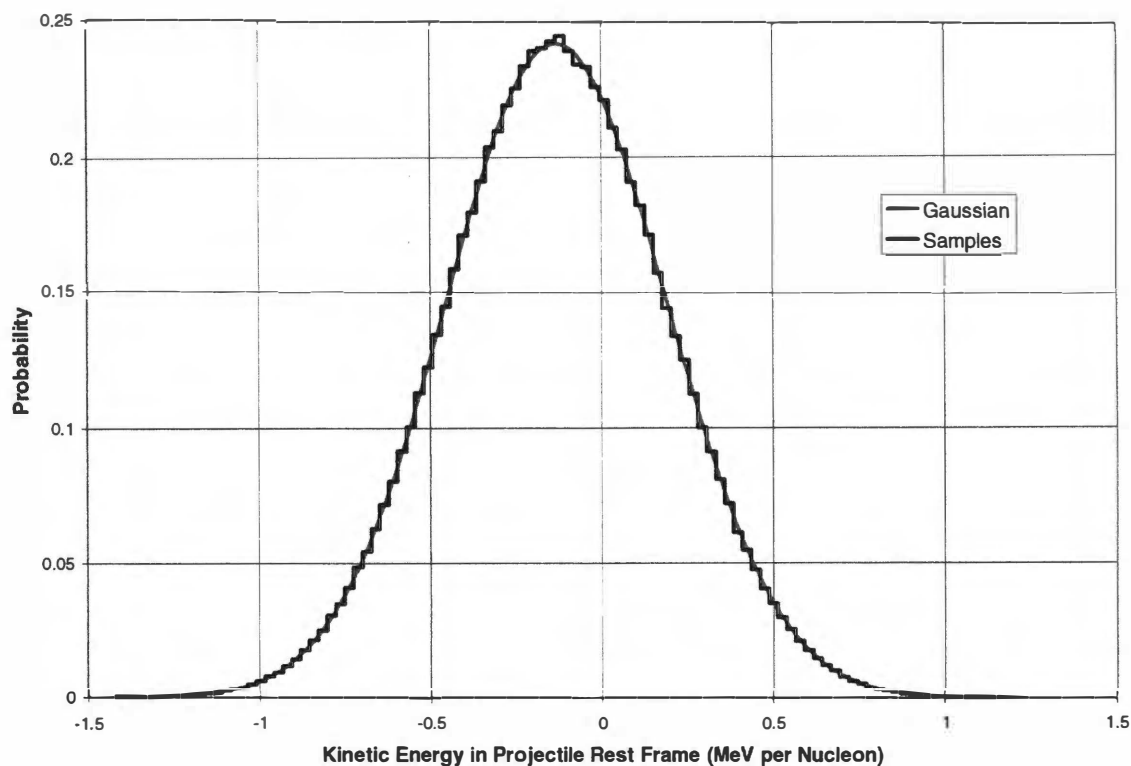


Figure 5.1: Fragment ${}^7\text{Li}$ Gaussian Kinetic Energy Distribution in the Projectile (${}^{12}\text{C}$) Rest Frame

Table 5.2: Event Generator Calculated Means and Standard Deviations for Fragment Kinetic Energy Distributions of ${}^{12}\text{C}$ at 1 GeV per nucleon on ${}^{12}\text{C}$

${}^{12}\text{C} + {}^{12}\text{C} \rightarrow \text{X} + {}^7\text{Li} + {}^3\text{He} + \text{p} + \text{n}$					
Charge	Mass	Mean	Standard Deviation	Event Generator Mean	Event Generator Stand. Deviation
3*	7*	974.1	62.87	983.5	58.76
2	3	934.5	109.7	950.0	65.96
1	1	795.5	179.3	833.8	146.7
0	1	794.6	179.6	812.4	137.3
*Fragment, i.e. remains of prefragment after ablation (MeV per nucleon)					

reminder, the event generator assumes the projectile is traveling in the Z direction. The X, Y, and Z momentum components of fragments emitted from the projectile were summed over one million inelastic collisions of ^{12}C at 1 GeV per nucleon on ^{12}C . Then these sums for each collision were averaged and the standard deviation of the sample for each direction was calculated. These mean value and standard deviation of each momentum component's sum are shown in Table 5.3.

Sample HETC-HEDS Results

The first comparison between HETC-HEDS and experiment compare fragment production in the forward and near forward directions. The first experiment measured fragments produced by 1050 MeV per nucleon ^{56}Fe on a 3.5 g/cm^2 graphite target (Stephens, 1997). The next two experiments also measure fragments produced by 1050 MeV per nucleon ^{56}Fe , but the targets were 5.0 g/cm^2 and 10.0 g/cm^2 graphite/epoxy composite (Stephens, 1997). These three experiments measured the fragment fluence for ions with charge number 25 through 12. A comparison of these experiments with HETC-HEDS can be seen in Figures 5.2, 5.3, and 5.4. In order to make a comparison with HETC-HEDS that considered all possible fragment charge numbers two more experiments was simulated. The first experiment measured fragments produced by 1037 MeV per nucleon ^{56}Fe on 1.39 g/cm^2 of Aluminum alloy 2219 followed by 0.54 g/cm^2 of Aluminum alloy 6061. A comparison of this experiment with HETC-HEDS can be seen in Figure 5.5 and Table 5.4. The second experiment measured fragments produced by

Table 5.3: Event Generator Calculated Means and Standard Deviations for Sums of Projectile Fragments' Momentum Components (^{12}C at 1 GeV per nucleon on ^{12}C)

Momentum Component	Mean of Resulting Momentum Component Sum	Standard Deviation of Resulting Momentum Components Sum
X	-9.78E-02	30.96364
Y	4.06E-01	75.07322
Z	-95.3355	80.43794

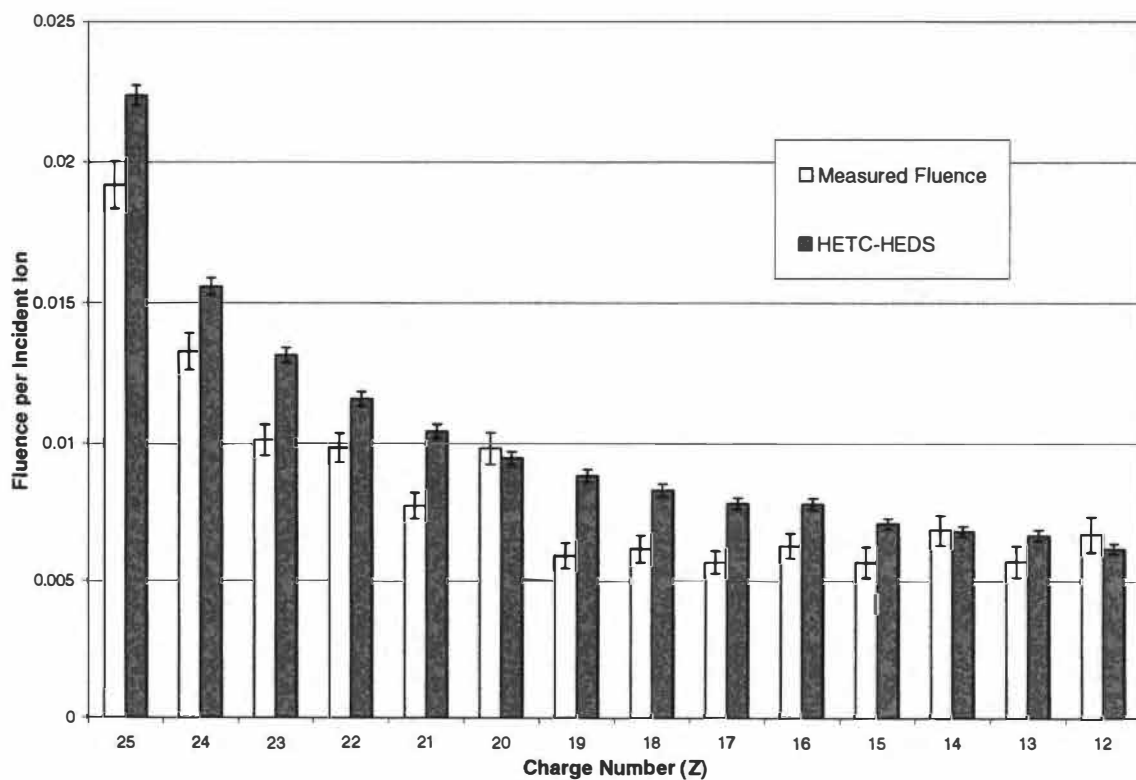


Figure 5.2: Fragment Fluence Due to 1050 MeV per Nucleon ^{56}Fe on 3.5 g/cm² of Graphite

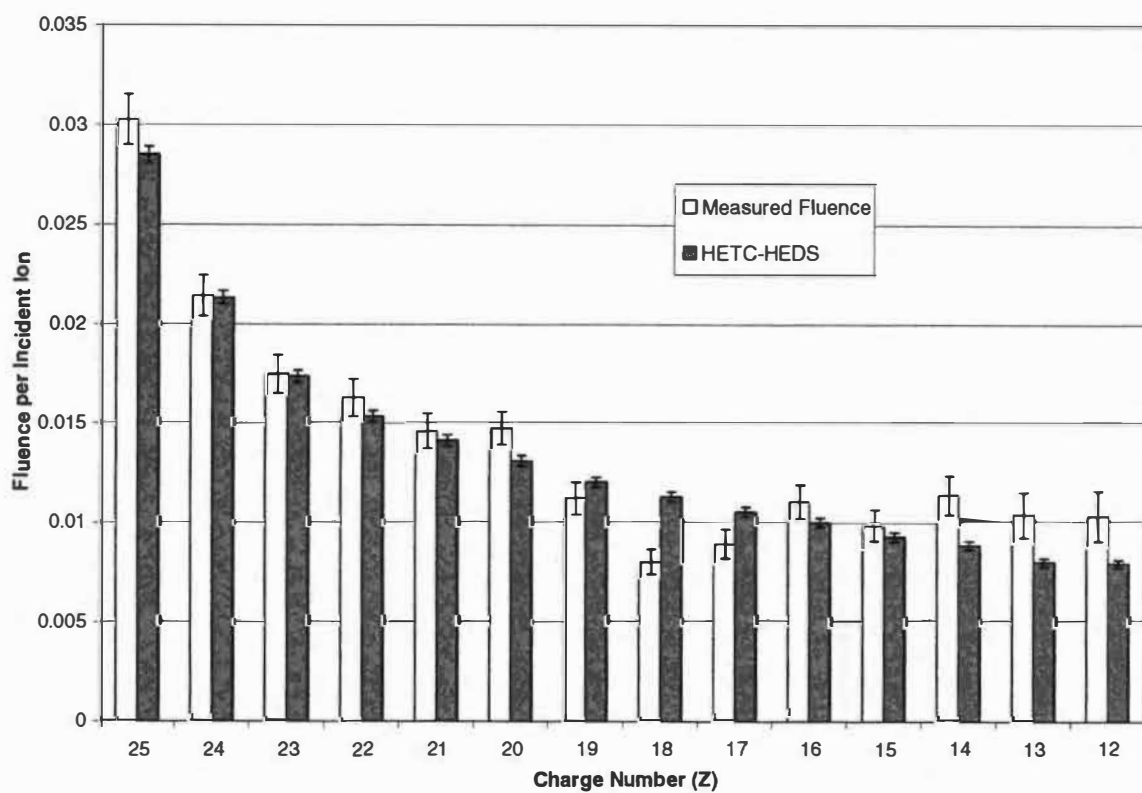


Figure 5.3: Fragment Fluence Due to 1050 MeV per Nucleon ^{56}Fe on 5 g/cm² of Graphite and Epoxy

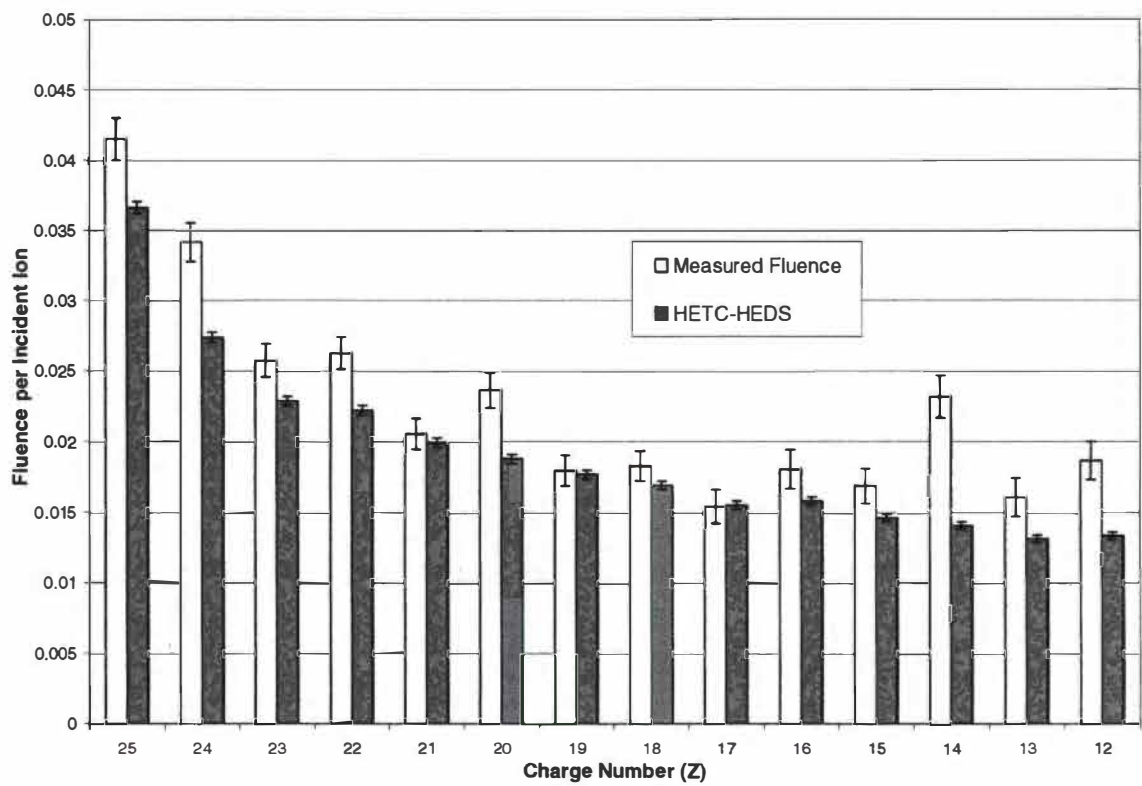


Figure 5.4: Fragment Fluence Due to 1050 MeV per Nucleon ^{56}Fe on 10 g/cm^2 of Graphite and Epoxy

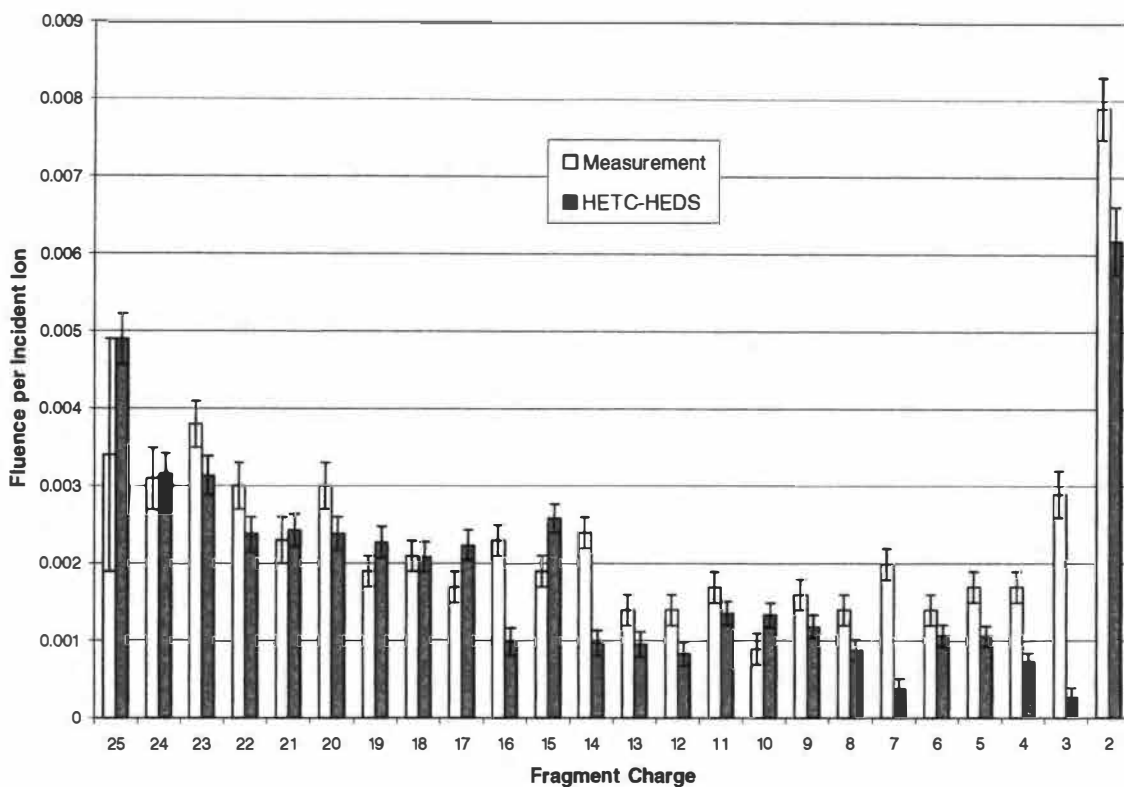


Figure 5.5: Fragment Fluence Due to 1037 MeV per Nucleon ^{56}Fe on 1.93 g/cm^2 of Aluminum Alloy

Table 5.4 Fragment Fluence Due to 1037 MeV per Nucleon ^{56}Fe on 1.93 g/cm^2 of Aluminum Alloy

Charge	Measured Fluence	Measured Fluence Error	HETC-HEDS Fluence	HETC-HEDS Fluence Error
26	0.9319	0.0012	0.9264	0.0039
1	0.0074	0.0004	0.6401	0.0059
0	0.0036	0.0003	0.7680	0.0069

1050 MeV per nucleon ^{56}Fe on 1.94 g/cm^2 of polyethylene. A comparison of this experiment with HETC-HEDS can be seen in Figure 5.6 and Table 5.5.

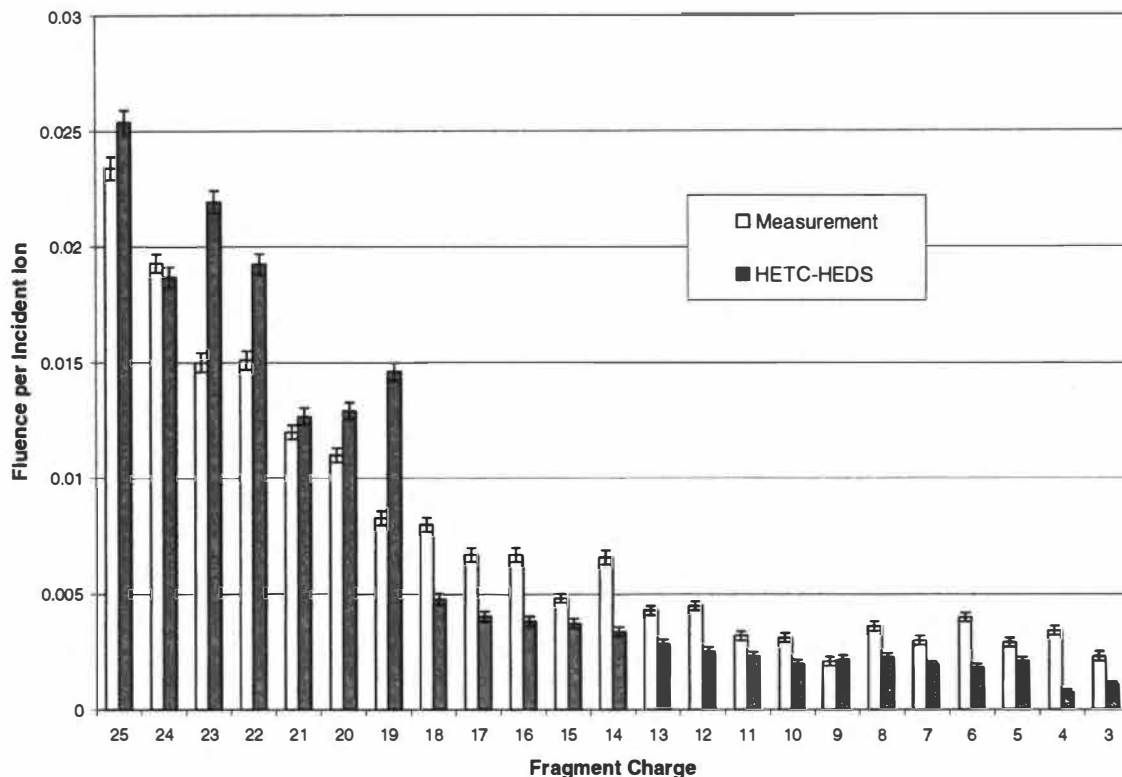


Figure 5.6: Fragment Fluence Due to 1050 MeV per Nucleon ^{56}Fe on 1.94 g/cm^2 of Polyethylene

Table 5.5 Fragment Fluence Due to 1050 MeV per Nucleon ^{56}Fe on 1.94 g/cm^2 of Polyethylene

Charge	Measured Fluence	Measured Fluence Error	HETC-HEDS Fluence	HETC-HEDS Fluence Error
26	0.7830	0.0005	0.7764	0.0052
2	0.0083	0.0003	0.0918	0.0010
1	0.0160	0.0004	1.5720	0.0049
0	0.0193	0.0004	1.8784	0.0053

VI. CONCLUSIONS & FUTURE WORK

Now that the results of several event generator and HETC-HEDS calculations have been presented in Chapter V a few comments are going to be made about them. This discussion is followed by a few suggestions to try to improve these specific results and to try and improve the event generator in general.

Discussion of Results

The three calculations carried out with the event generator were intended to try and duplicate results of the constituent models that make up the event generator, and therefore show that the models are working as expected inside the event generator. The first calculation done with the event generator, whose results are in Table 5.1, was an attempt to duplicate the results of the modified version of NUCFRG2 in Table 3.1. Comparing the cross sections listed in Table 5.1 one sees that the event generator is producing each fragment isotope at the correct rate.

Next, an attempt was made to duplicate the results of the modified version of the microscopic model for the estimation of energy degradation in nucleus-nucleus collisions listed in Table 3.3. First, one million samples of ${}^7\text{Li}$'s Gaussian kinetic energy distribution in the projectile rest frame were binned and plotted in Figure 5.1. Also in Figure 5.1 is the graph of a Gaussian distribution with the same mean and standard

deviation that was being used to sample ${}^7\text{Li}$'s kinetic energy. Figure 5.1 clearly shows that the Gaussian is being sampled properly. However, it must be pointed out that these samples were taken independent of any other fragments, so conservation of energy was not considered in these samples. Table 5.2 shows the average and standard deviation of the sample for one million samples of the kinetic energy distributions of the four fragments in the reaction channel being considered. These samples were all taken while considering conservation of energy. Comparing the results in Table 5.2 to the model predictions one sees that the mean and standard deviation of the sample calculated by the event generator is different from what the kinetic energy degradation model calculated. This difference is due to conservation of energy being implemented with a rejection method. This is also due to the fact that the kinetic energy degradation model calculates the mean and standard deviation for each fragment's Gaussian kinetic energy distribution without considering any of the other fragments. In this example neither of the limits established using the Fermi energy (equations (3.14) and (3.15)) were violated. However it is possible that the samples of the first three fragments' kinetic energies would make it impossible for any sample of the fourth fragment's kinetic energy distribution to conserve energy. At this point all the samples are rejected and the process starts again. Due to this rejection method samples will inevitably be thrown out and samples in the tails of the kinetic energy distributions may become even less likely to be chosen. This all leads to the differences observed in Table 5.2. However, it should be pointed out that the energies eventually chosen by this rejection method are a subset of the possible energies predicted by the kinetic energy degradation model. This can be seen in Table 6.1, which shows

Table 6.1: Domain of 99.9 Percent of Kinetic Energy Samples for the Kinetic Energy Degradation Model and the Event Generator

Charge	Mass	Kinetic Energy Degradation Model Domain		Event Generator Domain	
		$\mu - 3.29\sigma$	$\mu + 3.29\sigma$	$\mu - 3.29\sigma$	$\mu + 3.29\sigma$
3*	7*	767.3	1180.9	790.2	1176.8
2	3	573.6	1295.4	733.0	1167.0
1	1	205.6	1385.4	351.2	1316.4
0	1	203.7	1385.5	360.7	1264.1
*Remains of prefragment after ablation (MeV per nucleon)					

the mean plus and minus 3.29 standard deviations (99.9% confidence interval) for the kinetic energy degradation model and the event generator predictions.

The final calculation performed with the event generator considered the selection of scattering angles for projectile fragments and conservation of momentum in the projectile rest frame. It was stated earlier that projectile fragments are isotropically distributed in the projectile rest frame by the event generator. This is an approximation to the observation made by Morrissey that projectile like fragments are isotropically distributed in a frame moving nearly with the same velocity as the projectile. This implies that the net momentum components of fragments in the X, Y, and Z directions on the average should sum to zero. This would certainly be case in the frame that the fragments are truly isotropically distributed in. However, in the projectile rest frame this is not exactly true. The reason for this goes back to the sampling of kinetic energies. On the average fragments in the projectile rest frame have been downshifted in kinetic energy, i.e. their velocity is slower than that of the projectile. Therefore, on the average, more fragments in the projectile rest frame have momentum vectors that point in the negative Z direction (assuming the projectile was traveling parallel to the positive Z axis). This is illustrated in Table 5.3 where the average sum of momentum components in the X and Y directions is close to zero, but the average sum of the Z momentum component is less than zero.

Next five comparisons were made between HETC-HEDS and experimental measurements. The results of these comparisons are in Figures 5.2 through 5.5 and

Tables 5.4 and 5.5. In general HETC-HEDS did a good job of predicting the fragment fluences, especially for charge numbers closer to that of iron. As the charge number decreases the error between HETC-HEDS and the measurements increases. This is due in large part to the fact that NUCFRG2 tends to under predict production cross sections of fragments as the fragment charge number decreases. However, the agreement could be slightly improved by adding a coalescence model in order to form more light ions. Forming light ions by coalescence would also improve the agreement of neutron and proton production by reducing their numbers. It must be pointed out that the comparison of neutron, proton, and light ion production (up to fragment charge of 3 or 4) in these experiments and calculations is not exactly a direct comparison. In the actual experiments only the leading fragments were counted, meaning the heaviest particle that entered a detector as the result of a nucleus-nucleus collision was counted, while the remaining particles are ignored. In the HETC-HEDS calculation all particles that entered the detector were counted. This is not a concern except for protons, neutrons, and other light ions that may also result from a nucleus-nucleus collision along with the leading fragment. Since HETC-HEDS counted all light ions and nucleons entering the detector Figures 5.5 and 5.6 and Tables 5.4 and 5.5 are not comparing the same measurement for charge numbers 2, 1, and 0 (and possibly for charge numbers 3 and 4 due to light particle coalescence). However, it is encouraging that HETC-HEDS predicts more neutrons and protons than this experiment measured.

Suggested Future Work

One key improvement that this new event generator needs would affect a couple of its constituent models. When the event generator begins to simulate a nucleus-nucleus collision it needs to sample the impact parameter, which is the distance between the center of the projectile and the center of the target (and is discussed more in Appendix A). Currently, the modified version of NUCFRG2 samples the fragment, i.e. the remains of the prefragment after ablation, of the projectile and target regardless of impact parameter. For example, it is possible that the fragment of the projectile could be a neutron or proton, which translates into a central collision or impact parameter close to zero. However, the fragment of the target could be A_T-1 , which translates into a peripheral collision or an impact parameter close to the sum of the projectile and target radii. The microscopic model of kinetic energy degradation in nucleus-nucleus collisions is also dependent on the impact parameter. The manner in which momentum and energy is partitioned between the projectile spectator, participant, and target spectator is done by averaging over the impact parameter (equation (A.38)). If the correct impact parameter was known this averaging would not be necessary (equation (A.37)). Another discrepancy that could be removed is the definition of the number of nucleons in the projectile spectator, participant, and target spectator. Since the impact parameter in NUCFRG2 is not always consistent the number of participants may often vary between the impact parameters which are implied by choosing the projectile and target fragment. Only one number of projectile and target spectators will be calculated, but the impact

parameter required to have that many nucleons in the projectile and target spectator may not be the same. Therefore, when the projectile spectator, participant, and target spectator are partitioned in the kinetic energy degradation model a model different from NUCFRG2 is used, which is Glauber theory (equation (A.32)). If the impact parameter was consistent this could be removed and the number of nucleons in the projectile spectator, participant, and target spectator as calculated by NUCFRG2 could be used. There are two reasons that the impact parameter is currently not sampled. First, there is a lot of undocumented information in the NUCFRG2 model. Therefore, the methodology to calculate the number of nucleons in the projectile spectator, participants, and target spectator after sampling the impact parameter is not fully known. The second reason is that after the cross sections are calculated NUCFRG2 often multiplies certain cross sections by constants programmed into the code. It is assumed that these constants are used in order to make the code agree with experimental data more accurately. However, it is unclear how to involve these constants in a methodology where the impact parameter is being sampled.

Another issue that needs to be addressed is that fragments produced by the projectile or target are always emitted with no excitation energy. While this may often be correct it could possibly lead to incorrect ablated particle species. A light ion that is ablated may possibly leave the prefragment with some excitation energy. It is possible that excitation energy would be enough to alter the subsequent ablation products of the prefragment, and may even be enough to cause that fragment to subsequently ablate a particle itself.

Regardless, of whether or not the ablation products of the prefragment are altered the excitation energy remaining in each fragment needs to be quantified due to its effect on conservation of energy. This excitation energy could also lead to the emission of photons by fragments. Currently, photon emission is not modeled for the fragments or prefragment.

Another element that needs to be addressed which could affect conservation of energy, mass, and charge is meson production. Mesons are produced in nucleus-nucleus collisions, but are not currently modeled by the event generator. Each meson produced carries away kinetic energy, charge, mass, or some combination there of depending on the species of the meson. These particles need to be considered in order to better describe the nucleus-nucleus collision.

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APPENDICES

Appendix A

Appendix A-1: Additional Abrasion Ablation Theory

The number of nucleons removed through abrasion and ablation, ΔN , is a function of the impact parameter, b (Wilson et. al., 1994):

$$\Delta N = \Delta_{abr}(b) + \Delta_{abl}(b). \quad (\text{A.1})$$

The impact parameter is related to the impact separation radius, r , for a Coulomb trajectory:

$$b^2 = r(r - r_m), \quad (\text{A.2})$$

where

$$r_m = \frac{Z_p Z_T e^2}{E_{tot}}, \quad (\text{A.3})$$

Z_p is the atomic number of the projectile, Z_T is the atomic number of the target, E_{tot} is the total kinetic energy of the system in the center of mass frame, and

$$e^2 = 2R_y a_0, \quad (\text{A.4})$$

where R_y is the Rydberg constant and a_0 is the Bohr radius (Wilson et. al., 1994). In cases where b is large the interaction is dominated by Coulomb excitation. When b is small enough that the nuclear densities overlap, mass is removed from the projectile and target.

The number of nucleons removed through abrasion is:

$$\Delta_{abr} = FA_p \left[1 - e^{\frac{-C_T}{\lambda}} \right], \quad (\text{A.5})$$

where A_p is the nuclear mass number of the projectile and the nuclear mean free path is

$$\lambda = \frac{16.6}{E^{0.26}} \quad (\text{A.6})$$

with E defined as the projectile energy in MeV per nucleon (Wilson et. al., 1994). C_T is the target chord, at impact separation r from the projectile, parallel to the direction of travel of the projectile. When $r_T > r_P$, C_T is defined as (Wilson et. al., 1994):

$$C_T = \begin{cases} 2\sqrt{r_T^2 - x^2}, & x > 0 \\ 2\sqrt{r_T^2 - r^2}, & x \leq 0 \end{cases}, \quad (\text{A.7})$$

where

$$x = \frac{r_P^2 + r^2 - r_T^2}{2r}, \quad (\text{A.8})$$

r_P is the projectile radius and r_T is the target radius given by

$$r_{P,T} = 1.29\sqrt{r_{rms}^2 - 0.84^2}, \quad (\text{A.9})$$

and r_{rms} is the root-mean-square radius of the projectile or target taken from experimental data (De Vries, De Jager, and De Vries). When $r_P > r_T$, C_T is defined as (Wilson et. al., 1994):

$$C_T = \begin{cases} 2\sqrt{r_T^2 - x^2}, & x > 0 \\ 2r_T, & x \leq 0 \end{cases}, \quad (\text{A.10})$$

where

$$x = \frac{r_T^2 + r^2 - r_P^2}{2r}. \quad (\text{A.11})$$

The variable F , in equation (A.5), is the fraction of the projectile overlapping the target at impact separation r . When $r_T > r_P$, F is defined as (Wilson et. al., 1994):

$$F = 0.75 \left(\frac{1-\beta}{\nu} \right)^2 \sqrt{1-\nu} - 0.125 \left[3\sqrt{1-\nu} - 1 \right] \left(\frac{1-\beta}{\nu} \right)^3, \quad (\text{A.12})$$

where

$$\nu = \frac{r_P}{r_P - r_T}, \quad \beta = \frac{r}{r_P + r_T}, \quad \text{and} \quad \mu = \frac{r_T}{r_P}. \quad (\text{A.13})$$

If the collision is central then the projectile nucleus volume completely overlaps the target nucleus volume. So, if the collision is central and $r_T > r_P$, all the projectile nucleons are abraded, therefore $F = 1$ (Wilson et. al., 1994). When $r_P > r_T$, F is defined as (Wilson et. al., 1994):

$$F = 0.75 \left(\frac{1-\beta}{\nu} \right)^2 \sqrt{1-\nu} - 0.125 \times \left[\frac{3\sqrt{1-\nu}}{\mu} - \frac{\left[1 - \sqrt{(1-\mu^2)^3} \right] \sqrt{1-(1-\mu)^2}}{\mu^3} \right] \left(\frac{1-\beta}{\nu} \right)^3. \quad (\text{A.14})$$

If the collision is central and $r_P > r_T$ (Wilson et. al., 1994),

$$F = \left[1 - \sqrt{(1-\mu^2)^3} \right] \sqrt{1 - \left(\frac{\beta}{\nu} \right)^2}. \quad (\text{A.15})$$

The number of nucleons removed through ablation is (Wilson et. al., 1994):

$$\Delta_{abl} = \frac{E_s + E_x}{10} + \Delta_{spc}. \quad (\text{A.16})$$

Spectator nuclei are projectile nucleons that are outside of the interaction zone of an abrasion/ablation reaction; i.e. spectator nucleons do not overlap with the target nucleons during the collision. E_x is the excitation energy transferred across the projectile participant/spectator nuclei interface of an abrasion/ablation reaction,

$$E_x = 13C_l + \frac{1}{3} C_l (C_t - 1.5), \quad (\text{A.17})$$

where the second term only contributes if C_t is greater than 1.5 (Wilson et. al., 1994).

The longest chord in the projectile surface interface of the reaction is:

$$C_l = \begin{cases} 2\sqrt{r_P^2 + 2rr_T - r^2 - r_T^2}, & r > r_T \\ 2r_P, & r \leq r_T \end{cases}, \quad (\text{A.18})$$

which is the longest distance traveled by any target nucleon through the projectile (Wilson et. al., 1994). The maximum chord transverse to the projectile direction, which spans the projectile/target interface, is (Wilson et. al., 1994):

$$C_t = 2\sqrt{r_P^2 - b_P^2}, \quad (\text{A.19})$$

where

$$b_P = \frac{r_P^2 + r^2 - r_T^2}{2r}. \quad (\text{A.20})$$

The number of projectile spectator constituents is (Wilson et. al., 1994):

$$\Delta_{spc} = A_P F e^{-C_T/\lambda}. \quad (\text{A.21})$$

The excess surface area due to the abrasion part of an abrasion/ablation reaction removing nucleons from the colliding nuclei is (Wilson et. al., 1994):

$$\Delta S = 4\pi * r_P^2 \left(1 + P - \sqrt[3]{(1 - F)^2} \right). \quad (\text{A.22})$$

P is defined similarly to F. When $r_T > r_P$, P is defined as (Wilson et. al., 1994):

$$P = 0.125\sqrt{\mu\nu} \left(\frac{1}{\mu} - 2 \right) \left(\frac{1-\beta}{\nu} \right)^2 - 0.125 \left[0.5\sqrt{\mu\nu} \left(\frac{1}{\mu} - 2 \right) + 1 \right] \left(\frac{1-\beta}{\nu} \right)^3. \quad (\text{A.23})$$

If the collision is central then the projectile nucleus volume completely overlaps the target nucleus volume. Therefore, all the projectile nucleons are abraded. So, if the collision is central and $r_T > r_P$ all the projectile nucleons are abraded, therefore $P = -1$.

When $r_P > r_T$, P is defined as (Wilson et. al., 1994):

$$P = 0.125\sqrt{\mu\nu} \left(\frac{1}{\mu} - 2 \right) \left(\frac{1-\beta}{\nu} \right)^2 - 0.125 \times \left[0.5\sqrt{\frac{\nu}{\mu}} \left(\frac{1}{\mu} - 2 \right) - \left\{ \frac{\sqrt{1-\mu^2}}{\nu} - 1 \right\} \sqrt{\frac{2\mu-\mu^2}{\mu}} \right] \left(\frac{1-\beta}{\nu} \right)^3. \quad (\text{A.24})$$

If the collision is central and $r_P > r_T$ (Wilson et. al., 1994),

$$P = \left[\frac{\sqrt{1-\mu^2}}{\nu} - 1 \right] \sqrt{1 - \left(\frac{\beta}{\nu} \right)^2}. \quad (\text{A.25})$$

The excitation energy due to the distortion of the surface area in MeV is

$$E_s = 0.95 \times \Delta S \times f, \quad (\text{A.26})$$

where f is a semiempirical parameter defined as (Wilson et. al., 1994):

$$f = 1 + 5F + [1500 - 320(A_P - 12)]F^3. \quad (\text{A.27})$$

The third term in the equation for f makes no contribution unless the value inside of the square bracket is between 0 and 1500.

Next, the possible charge and mass of the resulting fragments must be determined. Charge is explicitly conserved

$$Z_P = Z_F + \Delta Z, \quad (\text{A.28})$$

where Z_P is the charge of the projectile, Z_F is the charge of the projectile fragment, and ΔZ is the total charged removed from the projectile in the abrasion/ablation reaction (Wilson et. al., 1994). The charge of the abraded nucleons (Z_{abr}) is proportional to the charge fraction of the projectile nucleus (Wilson et. al., 1994):

$$Z_{abr} = \frac{Z_P \Delta_{abr}}{A_P}. \quad (\text{A.29})$$

The total charge of the ablated nuclei (Z_{abl}) therefore is (Wilson et. al., 1994):

$$Z_{abl} = \Delta Z - Z_{abr}. \quad (\text{A.30})$$

Since the alpha particle is unusually tightly bound alpha production is maximized in the ablation process, so the number of alpha particles produced from ablation is:

$$N_\alpha = \left\{ \text{int}\left(\frac{Z_{abl}}{2}\right), \text{int}\left(\frac{A_{abl}}{4}\right) \right\}_{\min}, \quad (\text{A.31})$$

where $\text{int}(x)$ is the integer part of x (Wilson et. al., 1994). The remaining light ions, tritons, helium-3, and deuterons, are similarly maximized, each done so with the remaining ablated mass and charge in order of decreasing binding energy per nucleon (Wilson et. al., 1994).

Appendix A-2: Additional Fragment Kinetic Energy Distribution Theory

The microscopic model for the estimation of energy degradation in nucleus-nucleus collisions divides the collision system of two nuclei into three sources; A, the projectile spectator; B, the target spectator; and C, the participants. The mass number of the three sources is calculated using Glauber scattering theory (Glauber and Matthiae), and the equations for those mass numbers are (Tsao et. al.):

$$\begin{aligned}
 A &\approx A_p \left[1 - \frac{A_t^{2/3}}{(A_p^{1/3} + A_t^{1/3})^2} \right] \\
 B &\approx A_t \left[1 - \frac{A_p^{2/3}}{(A_p^{1/3} + A_t^{1/3})^2} \right] . \\
 C &= A_p + A_t - (A + B)
 \end{aligned} \tag{A.32}$$

The total momentum in the center of mass frame (i.e. $P_p + P_t = 0$) is partitioned as follows (Tsao et. al.):

$$\begin{aligned}
 P_A &= (1 - y) \frac{A}{A_p} P_p \\
 P_B &= (1 - y) \frac{B}{B_p} P_t . \\
 P_C &= -(P_A + P_B)
 \end{aligned} \tag{A.33}$$

In equation (A.33), y , which has the range $0 \leq y \leq 1$, is the parameter that controls the longitudinal degradation of the spectator. When y equals zero the spectators continue with their same momentum per nucleon. This is simply the straight ahead approximation. When y equals one all three sources move with the same velocity in the center of mass

frame (Tsao et. al.). Energy is partitioned between the three sources using the excitation energy per nucleon parameter, q (Tsao et. al.):

$$\begin{aligned} M_A &= A(m_n + xq) + V_A \\ M_B &= B(m_n + xq) + V_B \\ M_C &= C \left\{ m_n + \left[1 + \frac{A+B}{C}(1-x) \right] q \right\} + V_C \end{aligned} \quad , \quad (\text{A.34})$$

where m_n is the nucleon mass and V is the ground state mass excess. In equation (A.34), x , which also has a range $0 \leq x \leq 1$, is the parameter that controls the excitation energy between the three sources. When x equals zero source C receives all the excitation energy generated, and when x equals one the excitation energy is evenly distributed between the three sources (Tsao et. al.). When both x and y equal zero this simply is the straight ahead approximation, and when x and y both equal one the collision system is in equilibrium (Tsao et. al.). In order to calculate the excitation energy parameter q , conservation of energy in the center of mass frame is applied (Tsao et. al.):

$$E_p + E_t = E_A + E_B + E_C, \quad (\text{A.35})$$

where E is the total energy, i.e. $E_i^2 = P_i^2 + M_i^2$. Now equation (A.35) must be iterated to find the excitation energy parameter, $q = Q / (A_p + A_t)$, in equation (A.34). This is done in the following form (Tsao et. al.):

$$Q^{k+1} = Q^k + E_p + E_t - (E_A^k + E_B^k + E_C^k), \quad (\text{A.36})$$

where $Q^{k=0}$ equals zero. To this point the parameter x and y have been treated as impact parameter, b , dependent (Tsao et. al.):

$$\begin{aligned} x(b) &= x_0 \left[1 - \left(\frac{b}{b_m} \right)^2 \right] \\ y(b) &= y_0 \left[1 - \left(\frac{b}{b_m} \right)^2 \right] \end{aligned} \quad (\text{A.37})$$

where b_m is the maximum impact parameter, $b_m = R_t + R_p$, where R is the radius of the target or projectile. Averaging over the impact parameter gives (Tsao et. al.):

$$\begin{aligned} \bar{x} &= \frac{\Lambda}{2} x_0 \\ \bar{y} &= \frac{\Lambda}{2} y_0 \end{aligned} \quad (\text{A.38})$$

where Λ is the Lorentz parameter already define in equation (2.33). The values of $x_0 = 0.05$ and $y_0 = 0.25$ are taken from best fits to a large body of diverse accelerator data (Tsao et. al.).

The last additional piece of information needed is how to calculate $E_{\Delta A}$ in equation (2.30), which is the total energy of all the particles ablated by the prefragment or source A . Obviously, $E_{\Delta A} = M_{\Delta A} + KE_{\Delta A}$, where $\Delta A = A - A_f$ and $M_{\Delta A} = M_A - M_f$. M_f is the rest mass energy of the fragment and A_f is the mass number of the fragment. The kinetic energy of the ablated particles when A_f is less than or equal to A is given as (Tsao et. al.):

$$KE_{\Delta A}(A_f \leq A) = KE_A + \frac{3}{5} \epsilon_f + \epsilon_{coulomb}, \quad (\text{A.39})$$

where ϵ_f is the Fermi energy, taken to be 38 MeV, and $\epsilon_{coulomb}$ is the Coulomb barrier in the touching sphere approximation (Tsao et. al.):

$$\epsilon_{coulomb} = \frac{(Z-1)e^2}{r_0[\sqrt{A-1}+1]}, \quad (\text{A.40})$$

where $r_0 = 1.2$ fm, Z is the charge number of source A , and e^2 is the fine structure constant. When the mass number of the fragment, A_f , is larger than the source A a soft interaction is indicated. Therefore, the ablated particles are emitted from a compound nucleus formed by the entire projectile and target participants instead of source A (Tsao et. al.). The kinetic energy of the ablated particles is (Tsao et. al.):

$$KE_{\Delta A}(A_f > A) = KE_{comp} + \frac{3}{5}\epsilon_f + \epsilon_{coulomb}, \quad (\text{A.41})$$

where KE_{comp} is the kinetic energy of the compound nucleus (Tsao et. al):

$$KE_{comp} = \frac{(A_p - \Delta A)KE_p + (A_T - B)KE_A + \Delta A KE_A}{A_{comp}}, \quad (\text{A.42})$$

and A_{comp} is the mass number of the compound nucleus.

Here are a few more final notes concerning this model. In its initial form, when $A_f < A/2$, i.e. very light products, it is assumed that this light fragment was produced with a heavier fragment whose mass number is greater than $A/2$, and that the momentum per nucleon of the light fragment is the same as the heavy fragment (Tsao et. al). Also whenever the target, projectile, or both have a mass number less than 12 these data are scaled from the case when the target, projectile, or both are ^{12}C . The scaling factor is (Tsao et. al):

$$L = L_p L_t$$

$$L_p(A_p < 12) = \frac{6 + Z_p}{12} . \tag{A.43}$$

$$L_t(A_t < 12) = \frac{6 + Z_t}{12}$$

Appendix B: HETC-HEDS User's Manual

Appendix B-1: HETC-HEDS User's Manual

When setting up any problem with any radiation transport code there are three items that must be described, the problem geometry, the source, and the materials in the problem. This user's manual gives a description of how to input these three items into HETC-HEDS. Since HETC-HEDS was built on HETC the HETC user's manual (Gabriel et. al.) will often be referred to. This user's manual alone is not sufficient to run HETC-HEDS. The user must have the HETC manual to have a complete understanding of the code. Also included in this manual is some other general information about compiling and running HETC-HEDS and analyzing the output of HETC-HEDS. The following discussion is better illustrated by an example problem. Therefore, specific inputs are discussed in the context of a calculation comparing HETC-HEDS with the measurement of neutron spectra. The experimental measurements were made by Kurosawa et. al. and the experimental setup is described in the given reference (1999). The example herein will look at 400 MeV per nucleon carbon ions on a thick carbon target where neutron spectra were measured at 0, 7.5, and 15 degrees from the beam direction.

The HETC manual is part of the CALOR95 manual, and is located in Section 3 of the CALOR95 manual. The first issue addressed is the general HETC input and the material information needed (starting on p. 8). This information goes into an input file, which here is called `hetc.inp`. This file, as are all the others, is a fixed format file, and the HETC manual gives the required formatting. This is important because if the number is supposed to be a real number a decimal point must be present. Otherwise the number

will not be read correctly. The only exception to this is the number zero. This is also important because numbers must be input in the correct order with the correct spacing in fixed format files. A few important parameters that are included in this file are the geometry input file name; the history tape output file name; EMAX, the maximum particle energy allowed in the problem; ELOP, the proton energy cutoff; ELON, the neutron energy cutoff; MXMAT, the number of materials in the problem; MAXCAS, the number of source particles in one batch; MAXBCH, the number of source particle batches, and NHSTP, the unit number for the history tape whose name was listed earlier. Figure B.1 is the file hetc.inp that was created for the example being discussed. In hetc.inp the geometry file name is geom.inp and the history tape is hetc.dat, which is located in the directory /usr/scratch0/iontrans. Starting on line 10 of hetc.inp is the material information. Each material begins by providing the atom density (atoms/barn*cm) of hydrogen and the number of elements in the material excluding hydrogen. Looking at line 10 of hetc.inp one will see that material 1 has 0.048200 atoms/barn*cm of hydrogen and one other element beside hydrogen. Looking at line 11 one will see that the other element in material 1 is ^{12}C with an atom density of 0.039800 atoms/barn*cm. Material 9, beginning on line 31, contains no hydrogen, but does contain ten other elements. The three numbers on line 42 are the maximum dimensions of the problem geometry in the X, Y, and Z directions, respectively. The number on line 43 is a parameter needed for HETC, and no description is available.

```

1- geom.inp
2- /usr/scratch0/iontrans/hetc.dat
3- input for Kurasawa's data
4- 400 MeV carbon on c, al, cu, pb
5- 89997
6-      9600.      20.      20.00      9      10000      60      0
7-      1      -8      -1      11      0      9      2
8-      0.      1      1      1      0      -1
9-      0.0      0      5      0
10- 0.048200      1
11-      6.      12. 0.039800
12- 0.048200      1
13-      6.      12. 0.039800
14- 0.048200      1
15-      6.      12. 0.039800
16- 0.052300      1
17-      6.      12. 0.047400
18-      0.0      2
19-      6.      12. 0.114050
20-      6.      13. 0.001269
21-      0.0      1
22-      13.      27. 0.060307
23-      0.0      2
24-      29.      63. 0.058472
25-      29.      65. 0.026062
26-      0.0      4
27-      82.      204. 0.000462
28-      82.      206. 0.007945
29-      82.      207. 0.007286
30-      82.      208. 0.017275
31-      0.0      10
32-      7.      14. 3.898e-5
33-      7.      15. 1.447e-7
34-      8.      16. 1.049e-5
35-      8.      17. 4.255e-9
36-      8.      18. 2.103e-8
37-      18.      36. 7.84e-10
38-      18.      38. 1.47e-10
39-      18.      40. 2.321e-7
40-      6.      12. 7.409e-9
41-      6.      13. 8.24e-11
42-      82.      8.0      524.0
43- 15000.

```

Figure B.1: Hetc.inp

As was previously stated the geometry description of this problem is given in geom.inp, which is Figure B.2. The experimental geometry modeled in geom.inp is shown in Kurosawa's reference. It contains several detectors and the carbon target. The HETC manual begins to discuss the geometry input on the bottom of page 12. The geometry file is broken into three sections. First in geom.inp is the definition of all geometric bodies in the problem (similar to surface definitions in MCNP or body definitions in KENO). Table 1 on page 25 of the HETC manual provides all the required information needed for each possible body type in HETC. Next in geom.inp is the definition of the "cells" using the combinatorial geometry method. Finally, each "cell" is assigned to a zone and then each cell is assigned a material. To define a body in section one of geom.inp first list the three letter body type identifier, then give that body a number, and finally list the required geometric parameters. To define the cells using combinatorial geometry first give the cell a three letter name and then list the body numbers the cell is contained (+) or not contained (-) by (this is opposite MCNP's convention). For example, the cell named "102" on line 26 of geom.inp is inside body 6 and outside body 7. The geometry in HETC must always have a cell that contains the entire problem. In geom.inp the cell named "EV," defined as inside body 11 and outside all other bodies is the boundary of the geometry. Once a particle enters cell 11 its history ends. On line 35 of geom.inp all the cells are assigned a region number, and on line 36 of geom.inp all the cells are assigned a material number. The materials are numbered in the order in which they are listed in hetc.inp. The external void, cell 11 in this example, is material number 0, and any internal voids, none are given in this example, are material number 6666.

1-	0	0										
2-	RCC	1	0	0	0	0	0	0	0.01			
3-			1.5									
4-	RCC	2	0	0	0.01	0	0	0	0.05			
5-			1.5									
6-	RPP	3	-5.0	5.0	-5.0	5.0	10.06	30.06				
7-	RPP	4	-7.5	7.5	-7.5	7.5	510.06	510.56				
8-	RCC	5	0	0	510.56	0	0	12.7				
9-			6.35									
10-	BOX	6	57.8273	-7.5	506.7614	14.8717	0	-1.9579				
11-			0	15.	0	0.0653	0	0.4957				
12-	RCC	7	65.3282	0	506.2772	1.6577	0	12.5913				
13-			6.35									
14-	BOX	8	70.4013	-7.5	301.7789	14.4889	0	-3.8823				
15-			0	15.	0	0.1294	0	0.4830				
16-	RCC	9	77.7749	0	300.3197	3.2870	0	12.2673				
17-			6.35									
18-	RPP	10	-7.6	87.2958	-7.6	7.6	-0.1	523.36				
19-	RPP	11	-7.7	87.3958	-7.7	7.7	-0.2	523.46				
20-	END											
21-	Al		1									
22-	102		2									
23-	tar		3									
24-	102		4									
25-	213		5									
26-	102		6	-7								
27-	213		7									
28-	102		8	-9								
29-	213		9									
30-	air		10	-1	-2	-3	-4	-5	-6	-7	-8	
31-			-9									
32-	EV		11	-1	-2	-3	-4	-5	-6	-7	-8	
33-			-9	-10								
34-	END											
35-	1	1	1	1	1	1	1	1	1	1		
36-	6	4	5	4	1	4	2	4	3	9	0	

Figure B.2: Geom.inp

The source for HETC is defined in the subroutine SORS. In SORS nine parameters must be defined for each source particle. These parameters are energy, $e(1)$; particle species, $tip(1)$; particle weight, $wt(1)$; X position, $x(1)$; Y position, $y(1)$; Z position $z(1)$; X direction cosine, $u(1)$, Y direction cosine, $v(1)$, and the Z direction cosine, $w(1)$. Figure B.3 shows how these were defined in this example. As was stated before, the source particles are 400 MeV per nucleon ^{12}C ions. These ions strike the target evenly distributed inside a circle 1.5 cm in diameter. The geometry is oriented such that the ions are traveling parallel to the Z axis, and the center front face of the target is at the origin. Notice that the energy of the particle, $e(1)$, is in units of MeV not MeV per nucleon. The HETC manual gives the value of $tip(1)$ for protons, neutrons, etc on page 27. For ions heavier than protons:

$$tip(1) = (A * 1000) + Z. \quad (B.1)$$

Since these nine parameters are defined in a subroutine of HETC-HEDS they can be sampled arbitrarily. It is even possible to write additional subroutines to call in order to determine these initial source parameters. However, HETC-HEDS must be recompiled each time the source is changed.

Another important subroutine is INPUT, which locates all input and output files. This subroutine opens 6 files to be used as input and output. First, INPUT opens unit 5, which is usually reserved as input from the keyboard, and it names that unit `hetc.ppr`. Therefore, the file `hetc.ppr` discussed above must always be named `hetc.ppr` and be located in the same directory as the HETC-HEDS executable file, unless this open

```
e(1) = 4800.0
tip(1) = 12006.0
z(1) = sqrt(rand()) * 0.75
y(1) = 2 * 3.14159 * rand()
x(1) = z(1) * cos(y(1))
y(1) = z(1) * sin(y(1))
z(1) = 0.0
wt(1) = 1.0
u(1) = 0.0
v(1) = 0.0
w(1) = 1.0
```

Figure B.3: SORS

statement is changed and the program recompiled. INPUT also opens unit 6, which is usually reserved for output to the screen, HETC-HEDS names this `hetc.ppr`, so again to change the name and location of this file the subroutine must be changed and the program recompiled. Data files that are used by HETC-HEDS are units 1 and 3. If the location and/or name of these files are changed INPUT must be changed and recompiled as well. Unit 18 is the geometry input file, which the user provided the name and location of in `hetc.inp`. Finally, unit 9 is the history data tape. The user provides the name and location of this file in `hetc.inp` as well. To actually run HETC-HEDS simply type the name of the executable file at the command prompt.

Another parameter that is hard wired in HETC-HEDS is `abl` in subroutine REACTION. This parameter defines which ablation method is to be used by the nucleus-nucleus event generator in HETC-HEDS. In order to change the ablation method REACTION must be changed and recompiled.

Currently, HETC-HEDS is compiled by using the makefile utility. This is done because HETC-HEDS is not all in one file, so the makefile utility simplifies and speeds up the compiling process. To compile using the makefile utility simply type `make` at the command prompt in the directory that contains the makefile and all the parts of HETC-HEDS. One important thing to remember while compiling is to use the `-static` option. This option allows HETC-HEDS to leave a subroutine or function and upon its return all the variables are defined the same as when HETC-HEDS was last there. In other words,

HETC-HEDS does not reinitialize the variables in a subroutine or function. This compile time option is already built into the makefile.

As HETC-HEDS is running it writes information about each particle history on the history data tape. The types of events written to this file are listed on pages 27 and 28 of the HETC manual. A program, in this example named `analysis.f`, reads the data tape and can be changed to look for certain types of events, particle species, energies, angles, etc, or any desired combination of information on the data tape. The analysis program used to analyze the example that is currently being discussed is shown in Appendix B-2. The input file needed for the analysis program, `analysis.inp` in this example, is in Figure B.4. The input file contains the unit number of the history data tape (9), the batch number to begin the analysis at (1), the source particle number in each batch to begin the analysis at (1), the batch number to end the analysis at (60), the source particle number in each batch to end the analysis at (10000), and the name and location of the history data tape. The output file name in `analysis.f` in this example is `analysis.ppr`. The input and output names, unit 5 and 6 respectively, are defined in `analysis.f`. Therefore, to change these names `analysis.f` must be changed and recompiled.

The “do while” loop on line 57 of `analysis.f` is where the analysis program begins to count the neutrons that were produced at certain angles and energies. The first thing that is tested is `ncol`, which if equal to `-3` represent the end of a single batch, `1` represents the beginning of a new source particle (i.e. history), and `7` represents an internal boundary

9	1	1	60	10000
/usr/scratch0/iontrans/hetc.dat				

Figure B.4: Analysis.inp

crossing. The parameter `ncol` describes what type of event just occurred for the current particle. The possible values of `ncol` and their definitions are on pages 27 and 28 of the HETC manual. Next `tip` is tested to see if the particle crossing an internal boundary was a neutron, i.e. `tip` equal 1. There are three detectors in this problem detector 1 at 0 degrees, detector 2 at 7.5 degrees, and detector 3 at 15 degrees. These angles are measured from the Z axis or source particle direction. These three detectors are all NE213 liquid scintillators and each has a NE102A plastic scintillator in front of it. Detector 1 is material 1, detector 2 is material 2, and detector 3 is material 3, but material 1, 2, and 3 are all exactly the same. Material 4 models the NE102A detectors. At this point if a neutron crosses an internal boundary it is tested to see if it passes from material 4 (`mat` equal 4) to the next medium 1, 2, or 3 (`nmed` equal 1, 2, or 3). If one of these tests are passed the neutron is placed in the correct angular bin and next is tested to see what energy bin it should be placed in. Finally, `analysis.f` calculates the standard deviation of the mean for these results and prints the results to the output file. To compile `analysis.f` type “`f77 -static analysis.f`” and to run the executable file type “`a.out <analysis.inp>analysis.ppr.`”

Appendix B-2: Analysis.f

```
c this is for the non-rotated target calculations
c program to edit het collision tape
common/label/
1 nhst ,n,in,io,ncol,nocas,name,mat,nmed,lelem,nopart,nabov
2, nbelo,maxbch,maxcas,mxmat,ngroup,npidk,nicol,nquit,nexct
3,npart(6),nel(8),namea(300)
4 , x,y,z,xc,yc,zc,oldwt,wt,e,ec,u,v,w,tip,apr,zpr,erex,ex
5,hevsum,uu,emax,wtevap,zz(10,16),a(10,16),sigg(10,17),sigmx(7,17)
6,hsigg(5,17),tipa(300),ea(300),ua(300),va(300),wa(300),wta(300)
7,tib(300),eb(300),ub(300),vb(300),wb(300),wtb(300),epart(100,2)
8,emin(7),bold,blz,hepart(100,4)
c for the non-rotated target 1=0-deg 2=7.5-deg 3=15-deg
c for the rotated target 1=30-deg 2=60-deg 3=90-deg
dimension dl(43),d2(48),d3(50),sd1(43),sd2(48),sd3(50),e1(44),
xe2(49),e3(51),sum1(43),sum2(48),sum3(50),sumsq1(43),sumsq2(48),su
xmsq3(50)
character*4 namef(25)
data e1/828.7,719.634,566.2,510.6,450.5,401.9,361.9,320.8,287.1,2
x59,230.9,207.6,184.9,166,150,134.6,121.6,109.2,98.71,88.79,79.57,
x71.77,64.53,57.89,52.25,47.08,42.36,38.08,34.42,31.1,28.08,25.36,
x22.9,20.69,18.71,16.85,15.2,13.73,12.42,11.21,10.14,9.157,8.263/e
x2/991.8,861.5,761.1,681.1,587.2,514.9,457.3,410.3,359.6,318.9,285
x.6,257.7,228.8,204.9,184.9,164.8,148,131.6,118,106.4,95.31,85.9,7
x6.95,69.38,62.24,56.17,50.5,45.66,41.15,36.99,33.44,30.17,27.18,2
x4.46,21.99,19.89,17.98,16.25,14.68,13.27,12,10.82,9.761,8.819,7.9
x49,7.178,6.494,5.866,5.29407/e3/922.1,776.2,669.3,587.2,522.1,469
x,405.6,355.9,315.9,283,247.4,218.7,195.1,175.5,155.1,138.2,124.2,
x110.1,98.36,88.49,78.81,70.69,63.8,57.12,51.46,46.07,41.5,37.19,3
x3.53,30.1,27.18,24.46,21.95,19.81,17.85,16.05,14.51,13.11,11.83,1
x0.67,9.619,8.675,7.827,7.065,6.382,5.77,5.202,4.696,4.246,3.832,3
x.465/
open(unit=5,file='analysis.inp')
in =5
open(unit=6,file='analysis.ppr',status='old')
io =6
read(in,4) nhstp,nbch1,ncas1,nbch2,ncas2
4 format(5i10)
read(in,111) namef
111 format(25a4)
nhst = nhstp
open(unit=nhstp,file=namef,form='unformatted')
n = 0
nbch=1
nummax = 35
numbat = 0
do i=1,43,1
d1(i) = 0
sd1(i) = 0
sum1(i) = 0
sumsq1(i) = 0
enddo
do i=1,48,1
d2(i) = 0
sd2(i) = 0
sum2(i) = 0
sumsq2(i) = 0
enddo
do i=1,50,1
d3(i) = 0
sd3(i) = 0
sum3(i) = 0
sumsq3(i) = 0
enddo
```

```

do while(numbat.lt.nummax)
  call rednmt
  if(ncol.eq.-3)then
    numbat = numbat + 1
  elseif(ncol.eq.1)then
    do i=1,43,1
      sum1(i) = d1(i) - sum1(i)
      sumsq1(i) = sumsq1(i) + (sum1(i)*sum1(i))
    enddo
    do i=1,48,1
      sum2(i) = d2(i) - sum2(i)
      sumsq2(i) = sumsq2(i) + (sum2(i)*sum2(i))
    enddo
    do i=1,50,1
      sum3(i) = d3(i) - sum3(i)
      sumsq3(i) = sumsq3(i) + (sum3(i)*sum3(i))
    enddo
  elseif(ncol.eq.7)then
  c elseif(ncol.eq.4)then
  c elseif(ncol.eq.2)then
    if(tip.eq.1.)then
      if(mat.eq.4.and.nmed.eq.1)then
        if(ec.le.e1(1))then
          do i=2,44,1
            if(ec.gt.e1(i))then
              d1(i-1)=d1(i-1)+1
              goto 1
            endif
          enddo
        endif
      elseif(mat.eq.4.and.nmed.eq.2)then
        if(ec.le.e2(1))then
          do i=2,49,1
            if(ec.gt.e2(i))then
              d2(i-1)=d2(i-1)+1
              goto 1
            endif
          enddo
        endif
      elseif(mat.eq.4.and.nmed.eq.3)then
        if(ec.le.e3(1))then
          do i=2,51,1
            if(ec.gt.e3(i))then
              d3(i-1)=d3(i-1)+1
              goto 1
            endif
          enddo
        endif
      endif
    endif
  endif
1 enddo
  xnum = maxcas * numbat
  do i=1,43,1
    sum1(i) = d1(i) - sum1(i)
    sumsq1(i) = sumsq1(i) + (sum1(i)*sum1(i))
  enddo
  do i=1,48,1
    sum2(i) = d2(i) - sum2(i)
    sumsq2(i) = sumsq2(i) + (sum2(i)*sum2(i))
  enddo
  do i=1,50,1
    sum3(i) = d3(i) - sum3(i)
    sumsq3(i) = sumsq3(i) + (sum3(i)*sum3(i))
  enddo

```

```

do i=1,43,1
  sd1(i) = (sumsq1(i)/xnum) - ((d1(i)/xnum)*(d1(i)/xnum))
  sd1(i) = sd1(i) / (xnum - 1)
  sd1(i) = sqrt(sd1(i))
enddo
do i=1,48,1
  sd2(i) = (sumsq2(i)/xnum) - ((d2(i)/xnum)*(d2(i)/xnum))
  sd2(i) = sd2(i) / (xnum - 1)
  sd2(i) = sqrt(sd2(i))
enddo
do i=1,50,1
  sd3(i) = (sumsq3(i)/xnum) - ((d3(i)/xnum)*(d3(i)/xnum))
  sd3(i) = sd3(i) / (xnum - 1)
  sd3(i) = sqrt(sd3(i))
enddo
write(6,*) '0-degrees'
write(6,*)e1(1)
do i=1,43,1
  write(6,*)e1(i+1),d1(i)/xnum,sd1(i),d1(i)
enddo
write(6,*)
write(6,*) '7.5-degrees'
write(6,*)e2(1)
do i=1,48,1
  write(6,*)e2(i+1),d2(i)/xnum,sd2(i),d2(i)
enddo
write(6,*)
write(6,*) '15-degrees'
write(6,*)e3(1)
do i=1,50,1
  write(6,*)e3(i+1),d3(i)/xnum,sd3(i),d3(i)
enddo
stop
end

subroutine rednmt
c*****rednmt
c  reads output history tape from nmt
  common/label/
1  nhst ,n,in,io,ncol,nocas,name,mat,nmed,lelem,nopart,nabov
2  ,nbelo,maxbch,maxcas,mxmat,ngroup,npidk,nlcol,nquit,nexct
3  ,npart(6),nel(8),namea(300)
4  ,x,y,z,xc,yc,zc,oldwt,wt,e,ec,u,v,w,tip,apr,zpr,erec,ex
5  ,hevsum,uu,emax,wtevap,zz(10,16),a(10,16),sigg(10,17),sigmx(7,17)
6  ,hsigg(5,17),tipa(300),ea(300),ua(300),va(300),wa(300),wta(300)
7  ,tib(300),eb(300),ub(300),vb(300),wb(300),wtb(300),epart(100,2)
8  ,emin(7),bold,blz,hepart(100,4)
  nhstp = nhst
2  read(nhstp,end=2000)ncol,nocas,name,mat,nmed,x,y,z,xc,yc,zc,oldwt,
  1wt,e,ec,u
  1,v,w,tip,bold,blz,lelem,nopart,nabov,nbelo,apr,zpr,erec,ex,hevsum,
  2uu,(npart(i),i=1,6)
  ngo =ncol+5
  go to(10,10, 5,1, 5,10,20,20,10,20,80,10,10),ngo
5  call error
1  read(nhstp) maxbch,maxcas,mxmat,ngroup,npidk,nlcol,nquit,(emin(1)
  1,l=1,7),emax,nexct ,nsprd,nwsprd,nseudo,n
  read (nhstp) (nel(m),m=1,mxmat)
  do111 m=1,mxmat
  nelm = nel(m)
  read (nhstp) (zz(1,m),a(1,m),sigg(1,m),l=1,nelm)
  read (nhstp) (sigmx(i,m),i=1,7)
111 read (nhstp) (hsigg(i,m),i=1,5)
  mx = mxmat + 1
  read (nhstp) (sigmx(i,mx),i=1,7)
  write(io,60)

```

```

2 nhstp,      maxbch,maxcas,mxmat ,ngroup,npidk,nlcol,nquit,nexct
1 ,nsprcd,nwsprcd,nseudo,n,emax,(emin(1),l=1,7)
60 format(1h1,50x,' reading log. ',i2,' as nmt tape'
4           /1h0,20x,' maxbch maxcas mxmat n
lgroun npidk nlcol nquit nexite nsprcd nwsprcd nseudo nbe
1rtp'/18x
2,12i8/1h0,56x,'emax 'e12.4/1h0,50x,'cutoff energies for types 1-7'
3/22x,7e12.4)
do 70 m=1,mxmat
nelm = nel(m)
write(io,65) m,
1      (1,zz(1,m),a(1,m),sigg(1,m),l=1,nelm)
65 format(1h0,10x,'medium 'i4/1h0,13x,'nuclide no.      z no.
1a no.      ',26h'geometric' xsect (per cm)/(16x,i4, 6x,e12.4,2x,e12
2.4,9x,e12.4))
write(io,66) m, (sigmx(i,m),i=1,7)
66 format(1h0,15x,'transport xsects for particle types 1-7 in medium
1 ',i4,' in per cm'/15x,7e12.4/)
write(io,67) m, (hsigg(i,m),i=1,5)
67 format(1h0,15x,'max hydrogen xsects for particle types 1-5 in medi
lum ',i4,' in per cm'/15x,5e12.4/)
70 continue
10 return
20 if(nabov)100,40,30
30 read(nhstp,end=2000)(namea(i),tipa(i),ea(i),ua(i),va(i),wa(i),
1wta(i)
1, i=1,nabov)
40 if(nbelo)100,80,50
50 read(nhstp,end=2000)(tib(i),eb(i),ub(i),vb(i),wb(i),wtb(i),
1i=1,nbelo)
80 do 90 j=1,6
np=npart(j)
if(np)100,90,95
95 if(j-2)85,85,105
85 read(nhstp,end=2000) wtevap,(epart(k,j),k=1,np)
go to 90
105 l=j-2
110 read(nhstp,end=2000) wtevap,(hepart(k,l),k=1,np)
90 continue
go to 10
100 call error
2000 return
end
subroutine error
return
end

```

VITA

Thomas Martin Miller was born in Flowood, Mississippi, on April 18, 1977. He grew up in Meridian, Mississippi, and graduated from Meridian High School in May 1995. The following August he entered the University of Tennessee, Knoxville, and in May of 1999 received a Bachelor of Science degree in Nuclear Engineering, Magna Cum Laude. He entered the graduate school at the University of Tennessee, Knoxville, in August of 1999, and in May of 2001 he received a Master of Science degree in Nuclear Engineering. While working on his master's degree, he was employed by the Oak Ridge National Laboratory in the Computational Physics and Engineering Division. He assisted with the design of the Spallation Neutron Source while working at Oak Ridge. In August of 2001 he began working towards the Doctor of Philosophy degree in Nuclear Engineering at the University of Tennessee, Knoxville, which he completed in December of 2004. His dissertation research was sponsored by NASA's Marshall Space Flight Center in Huntsville, Alabama, through NASA's Graduate Student Research Program. After completion of his Doctorate degree he will begin working at the Bettis Atomic Power Laboratory in Pittsburgh, Pennsylvania, in the Shielding Design and Methods Development group.

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