A CLOSED FORM SOLUTION TO HZE PROPAGATION

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ABSTRACT

An analytic solution for high-energy heavy ion transport assuming straightahead and velocity conserving interactions with constant nuclear cross reactions is given in terms of a Green's function. The series solution for the Green's function is rapidly convergent for most practical applications. The Green's function technique can be applied with equal success to laboratory beams as well as to galactic cosmic rays allowing laboratory validation of the resultant space shielding code.
Introduction

Several approaches to the solution of high energy heavy ion propagation have been developed (1-12) over the last 20 years. All but one (5) have assumed the straightahead approximation and velocity conserving interactions. Only two (5, 8) have incorporated energy-dependent nuclear cross sections. The approach by Curtis et al. (1) for a primary ion beam represented the first generation secondary fragments as a quadrature over the collision density of the primary beam. Allkofer and Heinrich (2) used an energy multigroup method in which an energy-independent fragmentation transport approximation was applied within each energy group after which the energy group boundaries were moved according to continuous slowing down theory \(-\frac{dE}{dx}\). Chatterjee et al. (3) solved the energy-independent fragment transport equation with primary collision density as a source and neglecting higher-order fragmentation. The primary source term extended only to the primary ion range from the boundary. The energy-independent transport solution was modified to account for the finite range of the secondary fragment ions. Wilson (4) derived an expression for the ion transport problem to first order (first-collision term) and gave an analytic solution for the depth-dose relation. In ref. 5, the more common approximations used in solving the heavy ion transport problem were examined. The effects of conservation of velocity on fragmentation
and the straightahead approximation are found to be negligible for cosmic ray applications. Solution methods for representing the energy-dependent nuclear cross sections are developed. Letaw et al. (6) approximate the energy loss term and ion spectra by simple forms for which energy derivatives are evaluated explicitly (even if approximately). The resulting ordinary differential equations in position are solved analytically similar to the method of Allkofer and Heinrich (2). This approximation results in a decoupling of motion in space and change in energy. In Letaw's formalism, the energy shift is replaced by an effective attenuation factor. Wilson adds the next higher-order (second collision) term (7). This term was found to be very important in describing 670 MeV/amu $^{20}$Ne beams. The three-term expansion of ref. 7 was modified to include the effects of energy variation of the nuclear cross sections (8). The integral form of the transport equation (5) was further used to derive a numerical marching procedure to solve the cosmic ray transport problem (9). This method can easily include the energy-dependent nuclear cross sections within the numerical procedure. Comparison of the numerical procedure (9) with an analytical solution to a simplified problem (10) validates the solution technique to about 1 percent accuracy. Several solution techniques and analytic methods have been developed for testing future numerical solutions to the transport equation (11, 12). More recently, an analytic solution for
the laboratory ion beam transport problem has been derived assuming a straightahead approximation, velocity conservation at the interaction site, and energy-independent nuclear cross sections (13).

In the above overview of past developments, the applications split into two separate categories according to a single ion species with a single energy at the boundary versus a broad host of elemental types with a broad continuous energy spectrum. Techniques requiring a representation of the spectrum over an array of energy values require vast computer storage and computation speed for the laboratory beam problem to maintain sufficient energy resolution. On the other hand, analytic methods (5, 9) are probably best applied in a marching procedure (9) which again has within it a similar energy resolution problem. This is a serious limitation since we require a final HZE code for cosmic ray shielding which has been validated by laboratory experiments. In the present paper, we examine new methods which appear to overcome these difficulties.

**The HZE Transport Problem**

In moving through extended matter, heavy ions lose energy through interaction with atomic electrons along their trajectories. On occasion, they interact violently with nuclei of the matter producing ion fragments moving in the forward direction and low energy fragments of the struck target nucleus.
equations for the short-range target fragments can be solved in closed form in terms of collision density (ref. 5). Hence, the projectile fragment transport is the interesting unsolved problem. In previous work, the projectile ion fragments were treated as if all went straightforward. We continue with this assumption herein, noting that an extension of the beam fragmentation model to three dimensions is being developed (ref. 14).

With the straightahead approximation and the target secondary fragments neglected (ref. 5), the transport equation may be written as

\[ \frac{\partial}{\partial x} \left( \frac{\partial}{\partial E} \tilde{S}_j (E) + \sigma_j \right) \phi_j (x, E) = \sum_{k \neq j} m_{jk} \sigma_k \phi_k (x, E) \]  

where \( \phi_j (x, E) \) is the flux of ions of type \( j \) with atomic mass \( A_j \) at \( x \) moving along the \( x \)-axis at energy \( E \) in units of MeV/amu, \( \sigma_j \) is the corresponding macroscopic nuclear absorption cross section, \( \tilde{S}_j (E) \) is the change in \( E \) per unit distance, and \( m_{jk} \) is the fragmentation parameter for ion \( j \) produced in collision by ion \( k \). The range of the ion is given as

\[ R_j (E) = \int_0^E \frac{dE'}{\tilde{S}_j (E')} \]  

The solution to equation (1) is to be found subject to boundary specification at \( x = 0 \) and arbitrary \( E \) as
\[ \phi_j(0, E) = F_j(E) \]  

(3)

Usually \( F_j(E) \) is taken as an incident laboratory ion beam spectrum or the cosmic ray spectrum.

It follows from Bethe's theory that

\[ S_j(E) = \frac{A_p Z_j^2}{A_j Z_p^2} S_p(E) \]  

(4)

for which

\[ \frac{Z_j^2}{A_j} \rho_j(E) = \frac{Z_p^2}{A_p} \rho_p(E) \]  

(5)

The subscript \( p \) refers to proton. Equation (5) is quite accurate at high energy and only approximately true at low energy because of electron capture by the ion which effectively reduces its charge, higher-order Born corrections to Bethe's theory, and nuclear stopping at the lowest energies. Herein, the parameter \( v_j \) is defined as

\[ v_j = \frac{Z_j^2}{A_j} \]  

(6)

so that

\[ v_j \rho_j(E) = v_k \rho_k(E) \]  

(7)

Equations (6) and (7) are used in the subsequent development, and the energy variation in \( v_j \) is neglected. The inverse function of \( \rho_j(E) \) is defined as

\[ E = \rho_j^{-1}[ \rho_j(E) ] \]  

(8)

and plays a fundamental role subsequently.
Impulse Response

One form of Green's function is the impulse response corresponding to a $\delta$-like source term at the boundary. We therefore seek a solution of

$$\left[ \frac{\partial}{\partial x} - \frac{\partial}{\partial E} \tilde{S}_j (E) + \sigma_j \right] G_{jm} (x, E; E') = \sum_k m_{jk} \sigma_k G_{km} (x, E; E')$$

(9)

where the boundary condition is

$$G_{jM} (0, E; E') = \delta_{jm} \delta (E - E')$$

(10)

for which transport solution may be written as

$$\phi_j (x, E) = \sum_M \int_0^\infty G_{jM} (x, E; E') F_M (E') \, dE'$$

(11)

The solution to equations (9) and (10) is straightforward, even if tedious (4, 7, 13) and is arrived at using the method of characteristics (15). The solution is expressed as a series as

$$G_{jM} (x, E; E') = \sum_i G_{jM}^{(i)} (x, E; E')$$

(12)

where

$$G_{jM}^{(0)} (x, E; E') = \frac{1}{\tilde{S}_j (E)} \exp (-\sigma_j x) \delta_{jm} \delta \left[ x + R_j (E) - R_M (E') \right]$$

(13)
\[ G_{jm}^{(1)}(x, E; E') = \frac{1}{S_j(E)} m_{jm} \sigma_m \frac{v_j}{\sqrt{\frac{v_M}{v_j}}} \exp\left\{ - \frac{1}{2} \sigma_j [x - R_j(E) - \eta'] \right\} \]

so long as

\[ \frac{v_M}{v_j} \left[ R_M(E') - x \right] < R_j(E) < \frac{v_M}{v_j} \left[ R_j(E) + x \right] \]

where

\[ \eta' = \frac{2v_M - R_M(E')}{v_M - v_j} - \frac{v_M + v_j}{v_M - v_j} \left[ R_j(E) + x \right] \]

Otherwise \( G_{jm}^{(1)}(x, E; E') \) is zero. After a complicated but straightforward manipulation, a similar result may be obtained \( G_{jm}^{(2)}(x, E; E') \) as

\[ G_{jm}^{(2)}(x, E; E') = \sum_k \frac{\sigma_{jk} \sigma_{kM} v_j}{S_j(E) \sqrt{\frac{v_M - v_k}{\Delta_{jkM}}}} e^{-\left( -\sigma_k x_{Mj} - \sigma_k x_{kl} - \sigma_j x_{jl} - \sigma_k x_{kM} - \sigma_k x_{ku} - \sigma_j x_{ju} \right)} \]

where \( x_{Mj} \), \( x_{kl} \), \( x_{Mj} \), and \( x_{kl} \) are values of \( x_M \) and \( x_k \) evaluated at the corresponding upper and lower limits of \( x_j \) and

\[ x_M = \left[ v_M R_M(E') - v_k (R_k(E) + x) + (v_k - v_j) x_j \right] / (v_M - v_k) \]

\[ x_k = \left[ v_M (R_M(E) + x) - v_M R_M(E') - (v_M - v_j) x_j \right] / (v_M - v_k) \]
The requirements that \( x_M \) and \( x_k \) be bounded by the interval \( 0 \) to \( x-x_j \) yields

\[
\begin{pmatrix}
0 & \leq x_j \leq x \\
\frac{v_k \left[ R_k(E) + x \right] - v_M R_M(E)}{v_k - v_j} & \frac{v_M \left[ R_M(E) + x \right] - v_M R_M(E)}{v_M - v_j}
\end{pmatrix}
\]

as the appropriate limiting values in equation (17) when \( v_M > v_k > v_j \). In the above brace, we always choose the most restrictive value for the limit. The requirement of equation (20) also implies the result that

\[
R_M^{-1} \left[ R_M(E) - x \right] \leq E \leq R_k^{-1} \left[ \frac{v_M R_M(E) - v_j x}{v_k} \right]
\]

as the range over which the result of equation (17) is not zero. In the event that \( v_k > v_M > v_j \), then

\[
\begin{pmatrix}
0 & \leq x_j \leq x \\
\frac{v_M \left[ R_M(E) + x \right] - v_M R_M(E)}{v_M - v_j} & \frac{v_M \left[ R_M(E) + x \right] - v_M R_M(E)}{v_M - v_j}
\end{pmatrix}
\]

As a result of equation (22)

\[
R_k^{-1} \left[ \frac{v_M R_M(E)}{v_k} - x \right] \leq E \leq R_M^{-1} \left[ \frac{R_M(E) - v_j x}{v_M} \right]
\]

In the event that \( v_M > v_j > v_k \), it follows that
\[ 0 \leq x_j \leq \begin{cases} \frac{x}{v_M \left[ R_M(E) + x - R_M(E') \right] / (v_M - v_j)} \\ \left[ v_M R_M(E') - v_k R_k(E) - v_k x \right] / (v_j - v_k) \end{cases} \]

where the lesser of the three values in the brace is used as the upper limit of \( x_j \) for which \( G^{(2)} \) of equation (17) is not zero. As a result of equation (24)

\[ R_M^1 \left[ R_M(E) - x \right] \leq E \leq R_k^{-1} \left[ \frac{v_M}{v_k} R_M(E') - x \right] \] (25)

Note that

\[ \Delta_{jkM} = \sigma_j + \left[ \frac{(v_k - v_j)}{(v_M - v_k)} \sigma_M - \frac{(v_M - v_j)}{(v_M - v_k)} \sigma_k \right] \]

Higher-order terms are similarly derived. Approximate expressions have been obtained as

\[ G_{j,M}^{(n)} (x, E; E') = \sum_{k, j_1, \ldots, j_{n-2}} \sigma_j \sigma_{j_1} \ldots \sigma_{j_{n-2}} M \quad g(j, k, j_1, \ldots, j_{n-2}, M) / (E_{ju} - E_{jl}) \] (27)

where

\[ E_{jl} = \begin{cases} R_M^1 \left[ R_M(E) - x \right] \quad v_M > v_k > v_j \\ R_k^{-1} \left[ \frac{v_M}{v_k} R_M(E') - x \right] \quad v_k > v_M > v_j \\ R_M^{-1} \left[ R_M(E') - x \right] \quad v_M > v_j > v_k \end{cases} \] (28)

and

\[ E_{ju} = \begin{cases} R_k^{-1} \left[ \frac{v_M}{v_k} R_M(E') - v_j x \right] / v_k \quad v_M > v_k > v_j \\ R_M^{-1} \left[ R_M(E) - v_j x / v_M \right] \quad v_k > v_M > v_j \\ R_k^{-1} \left[ \frac{v_M}{v_k} R_M(E') - x \right] \quad v_M > v_j > v_k \end{cases} \] (29)
and the g-functions of \( n + 1 \) arguments are defined as

\[
g(j_1) = \exp(-\sigma_{j_1} x)
\]

\[
g(j_1, j_2, \ldots, j_{n+1}) = \frac{g(j_1, j_2, \ldots, j_{n-1}, j_n) - g(j_1, j_2, \ldots, j_{n-1}, j_{n+1})}{\sigma_{j_{n+1}} - \sigma_{j_n}}
\]

The expression for \( G_{jM}^{(n)} \) given by equation (27) is taken as zero unless

\[
E_{ji} \leq E \leq E_{ju}
\]

Portions of the Green's function are shown for incident \(^{20}\)Ne beams at \( E' = 600 \text{ MeV/amu} \) at \( x = 20 \text{ cm} \) in figures 1 to 3. The contribution from \( G^{(1)} \) is shown as the solid curve, \( G^{(1)} + G^{(2)} \) is shown as the dash-dot curve, and \( G^{(1)} + G^{(2)} + G^{(3)} \) is shown as the dashed curve. The dash-double-dot curve representing the inclusion of \( G^{(4)} \) in the sum can hardly be distinguished signifying convergence to a high degree of accuracy. A fuller presentation of the Green's function for \(^{16}\)O fragments is given in figure 4, and a presentation of the \(^{12}\)C Green's function is given in figure 5. From the present result, the solution for any arbitrary boundary condition may be found using equation (11).

Although the present formalism presents a closed form solution for the more common form of the HZE propagation problem, many tasks remain before the HZE propagation problem is adequately solved. The inclusion of energy-dependent nuclear cross sections is known to be very important in obtaining accurate solutions.
to some problems (16). Treating the momentum spread of the fragments is more complicated for the higher-order terms. The inclusion of the light fragment spectra is a difficult challenge (17). Finally, the three-dimensional aspects of the problem have only partially been treated (14). Even these shortcomings of the HZE propagation problem remain without the mention of uncertainties in nuclear cross sections (18) or atomic/molecular cross sections. Clearly much work remains.
References


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FIGURE CAPTIONS

Fig. 1 - Sequence of approximations of the $^{170}$ flux spectrum after 20 cm of water for first order (-), second order (- - -), third order (---), and fourth order (-----) theories.

Fig. 2 - Sequence of approximations of the $^{160}$ flux spectrum after 20 cm of water for first order (-), second order (- - -), third order (--), and fourth order (-----) theories.

Fig. 3 - Sequence of approximations of the $^{12}$C flux spectrum after 20 cm of water for first order (-), second order (- - -), third order (--), and fourth order (-----) theories.

Fig. 4 - Green's function for $^{16}$O flux spectrum response to a 600 MeV/amu $^{20}$Ne flux at the boundary.

Fig. 5 - Green's function for $^{12}$C flux spectrum response to a 600 MeV/amu $^{20}$Ne flux at the boundary.