ANALYSIS OF THE THEORY OF HIGH-ENERGY ION TRANSPORT

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16. Abstract

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SUMMARY

In the operation of commercial high-altitude aircraft and manned spacecraft, exposure to the heavy-ion radiations of space must be considered. There is a need, therefore, to understand the interaction of these radiations with the structures and shielding materials of these transport vehicles. The development of analytical methods to study the transport properties of high-energy ions in materials is the topic of the present report.

Procedures for the approximation of the transport of high-energy ions are discussed on the basis of available data on ion nuclear reactions. A straightahead approximation appears appropriate for space applications. The assumption that the secondary-ion-fragment velocity is equal to that of the fragmenting nucleus is found to be inferior to straightahead theory but may be of sufficient accuracy if the primary ions display a broad energy spectrum. An iterative scheme for the solution of the inhomogeneous integral transport equations holds promise for practical calculation. A model calculation shows that multiply charged ion fragments (atomic number greater than 3) are able to penetrate to greater depths in comparison with the free path of a primary heavy ion (atomic number approximately equal to 25).

INTRODUCTION

The prospect of extensive space operations in the era of the Space Transportation System, of ever increasing altitude range of commercial aircraft operations, and of recent development of high-energy heavy-ion accelerators (especially in the context of radiotherapy) accentuates the need for a theoretical understanding of the interaction of energetic heavy ions with extended matter. The main limits on such developments in the past have been a result of the scarcity of information on the nuclear reactions induced by heavy-ion collisions (ref. 1). With the advent of the acceleration of heavy ions to relativistic energies by particle accelerators (refs. 2 and 3), needed experimental data will be forthcoming and the further development of heavy-ion transport theory now seems appropriate. In addition, progress in heavy-ion reaction theory is likewise being made (refs. 4 to 10); many of the transport parameters may be accurately estimated and implications of heavy-ion dynamics on the transport theory can now be investigated.

It is considered that the simplest approach to studying high-energy ion transport would be to implement the Monte Carlo method. However, as a result of the large number of possible outcomes of heavy-ion nuclear reactions, it is felt that inordinately large samples will be required to adequately represent even the more important quantities of the transport process. For this reason, the development of analytical methods appears to be a potentially fruitful area of research.

The purpose of the present paper is to make a preliminary analysis of heavy-ion transport theory with particular attention to the development of analytical methods well suited to numerical approximation without recourse to Monte Carlo methods (ref. 11). Since radiation protection is of concern, consideration will be given to evaluation of factors closely related to biological response (ref. 12).

SYMBOLS

A_j atomic mass of type j ion, amu

E ion kinetic energy, MeV/amu

$f_{jk}(E,E',\vec{\Omega},\vec{\Omega}')$ probability density of type k projectile with energy E' and motion along $\vec{\Omega}'$ to produce type j ion with energy in dE about E and in $d\vec{\Omega}$ about $\vec{\Omega}$, $(\text{sr-MeV/amu})^{-1}$

$G_j(\vec{x},\vec{\Omega},E)$ source of type j ions at $\vec{x}$ with energy E and direction $\vec{\Omega}$, $(\text{sr-cm}^3\text{-MeV/amu})^{-1}$

m nucleon mass, amu

$\vec{n}(\vec{r})$ outward directed unit normal vector at point $\vec{r}$ on bounding surface

$P_j(E)$ total survival probability of type j ion of energy E

$R_j(E)$ continuous slowing-down range of type j ion of energy E, cm

$r_{jk}(E,E',\vec{\Omega},\vec{\Omega}')$ double differential cross section for production of type j ions of energy E into direction $\vec{\Omega}$ by type k ions of energy E' from direction $\vec{\Omega}$, $(\text{cm-sr-MeV/amu})^{-1}$

$S_j(E)$ stopping power or linear energy transfer (LET) due to interaction of type j ion with orbital electrons of transport medium, MeV/cm

s,t	two-parameter net defined over bounding surface
x	one-dimensional position vector, g/cm^2
$\vec{x}$	position vector (see fig. 1), cm
$\vec{x}_n$	component of $\vec{x}$ perpendicular to $\vec{\Omega}$, cm
$\vec{\Gamma}_{\Omega,x}$	position vector defining point on boundary which is origin of vector connecting boundary to $\vec{x}$ along direction $\vec{\Omega}$ (see fig. 1), cm
$\vec{\gamma}(s,t)$	two-parameter vector function defining the bounding surface, cm
$\nu_{jk}(E)$	multiplicity of type j ions produced by collision of type k ion of energy E
ξ_j, η_j	characteristic coordinates of type j ion, cm
ρ	projection of $\vec{x}$ onto $\vec{\Omega}$, cm
$\Sigma_j(E)$	macroscopic absorption cross section for type j ion of energy E, cm^{-1}
σ_{jk}	standard deviation of momentum of type j ions produced in collision of type k ions, MeV/c
$\phi_j(\vec{x},\vec{\Omega},E)$	differential flux of type j ions at $\vec{x}$ directed toward $\vec{\Omega}$ with energy E, $(cm^2\text{-sec-sr-MeV/amu})^{-1}$
$\vec{\Omega}$	ion direction of motion

Superscripts:

P	projectile
T	target

Primes indicate a variable of summation or integration.

TRANSPORT THEORY

A heavy ion, after entering a region filled with ordinary matter, interacts with orbital electrons, causing ionization and excitation of the medium. Because of the large mass difference between the ion and these orbital electrons, only a small amount of the ion energy can be transferred in a collision with a single electron. As a result of the long range of the Coulomb force and the large percentage of the material volume occupied by electrons, the electron interactions can, to a good approximation, be treated as a continuous slowing-down process over any finite path length. Although the energy lost by an ion over some fixed path length fluctuates about a mean value, this fluctuation amounts to no more than a few percent (refs. 13 and 14) and is of no importance in the study of space radiation (ref. 15). In the following, continuous slowing-down theory will be assumed throughout and the relevant quantity is the average energy loss per unit path length, denoted by $S_j(E)$, where E is the ion energy and j denotes the ion type.

The mean free path for nuclear collisions is large (more than a centimeter); by comparison, the mean free path for collision of the ion with electrons is small. Whereas collisions with electrons result only in a small transfer of energy compared with the total ion kinetic energy, the nuclear collision generally alters (loss of mass and charge) the ion and the struck nucleus, with many secondary particles being produced. The secondary particles produced as fragments of the primary heavy ion will have longer ranges and free paths causing much greater penetration. As the secondaries undergo additional nuclear reactions, more secondaries, which penetrate deeper into the material, are produced. The purpose here is to develop the theoretical understanding of the transport of such radiations in extended materials.

The heavy-ion transport equations are derived by balancing the change in the ion flux as it crosses a small volume of material with the gains and losses due to nuclear collision (ref. 11). The resulting equations for a homogeneous material are given by

$$\left[\vec{\Omega} \cdot \nabla - \frac{1}{A_j} \frac{\partial}{\partial E} S_j(E) + \Sigma_j(E) \right] \phi_j\left(\vec{x}, \vec{\Omega}, E\right)$$

$$= \sum_k \int dE' \, d\vec{\Omega}' \, r_{jk}\left(E, E', \vec{\Omega}, \vec{\Omega}'\right) \phi_k\left(\vec{x}, \vec{\Omega}', E'\right) \tag{1}$$

where $\phi_j\left(\vec{x}, \vec{\Omega}, E\right)$ is the flux of ions of type j with atomic mass A_j at $\vec{x}$ with motion along $\vec{\Omega}$ and energy E in units of MeV/amu, $\Sigma_j(E)$ is the corresponding macroscopic cross section, $S_j(E)$ is the linear energy transfer (LET), and

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$r_{jk}(E,E',\vec{\Omega},\vec{\Omega}')$ is the production cross section for type j ions with energy E and direction $\vec{\Omega}$ by the collision of a type k ion of energy E' and direction $\vec{\Omega}'$. The term on the left side of equation (1) containing $S_j(E)$ is a result of the continuous slowing-down approximation, while the remaining terms of equation (1) are seen to be the usual Boltzmann terms. The solutions to equation (1) exist and are unique in any convex region for which the inbound flux of each ion type is specified everywhere on the bounding surface. If the boundary is given as the loci of the two-parameter vector function $\vec{\gamma}(s,t)$ for which a generic point on the boundary is given by $\vec{\Gamma}$, then the boundary condition is specified by requiring the solution of equation (1) to satisfy

$$\phi_j(\vec{\Gamma},\vec{\Omega},E) = \psi_j(\vec{\Gamma},\vec{\Omega},E) \tag{2}$$

for each value of $\vec{\Omega}$ such that

$$\vec{\Omega} \cdot \vec{n}(\vec{\Gamma}) < 0 \tag{3}$$

where $\vec{n}(\vec{\Gamma})$ is the outward directed unit normal vector to the boundary surface at the point $\vec{\Gamma}$ and ψ_j is a specified boundary function.

Equation (1), with the boundary condition (eq. (2)), may be written as an inhomogeneous integral equation. To do so requires inversion of the differential operator contained in brackets on the left-hand side of equation (1). As will be shown, there is a characteristic space in which the inversion is simplified. The transformation of equation (1) to this characteristic space will now be made. (See ref. 11 for a more detailed discussion.) Let the secondary particle source term on the right-hand side of equation (1) be denoted by $G_j(\vec{x},\vec{\Omega},E)$, so that

$$\left[\vec{\Omega} \cdot \nabla - \frac{1}{A_j}\frac{\partial}{\partial E} S_j(E) + \Sigma_j(E)\right] \phi_j(\vec{x},\vec{\Omega},E) = G_j(\vec{x},\vec{\Omega},E) \tag{4}$$

Multiplying equation (4) from the left by $S_j(E)$ results in

$$\left[\vec{\Omega} \cdot \nabla - \frac{S_j(E)}{A_j}\frac{\partial}{\partial E} + \Sigma_j(E)\right] \bar{\phi}_j(\vec{x},\vec{\Omega},E) = \bar{G}_j(\vec{x},\vec{\Omega},E) \tag{5}$$

where

$$\bar{\phi}_j(\vec{x},\vec{\Omega},E) = S_j(E)\, \phi_j(\vec{x},\vec{\Omega},E) \tag{6}$$

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and

$$\overline{G}_j\left(\vec{x},\vec{\Omega},E\right) = S_j(E)\, G_j\left(\vec{x},\vec{\Omega},E\right) \tag{7}$$

A set of characteristic variables are found to be

$$\rho = \vec{\Omega} \cdot \vec{x} \tag{8}$$

$$\vec{x}_n = \vec{x} - \rho\vec{\Omega} \tag{9}$$

$$\eta_j = \rho - R_j(E) \tag{10}$$

$$\xi_j = \rho + R_j(E) \tag{11}$$

and the new functions in this characteristic space are defined as

$$\chi_j\left(\eta_j,\xi_j,\vec{x}_n,\vec{\Omega}\right) = \overline{\phi}_j\left(\rho\vec{\Omega} + \vec{x}_n,\vec{\Omega},E\right) \tag{12}$$

$$g_j\left(\eta_j,\xi_j,\vec{x}_n,\vec{\Omega}\right) = \overline{G}_j\left(\rho\vec{\Omega} + \vec{x}_n,\vec{\Omega},E\right) \tag{13}$$

$$\overline{\Sigma}_j\left(\eta_j,\xi_j\right) = \Sigma_j(E) \tag{14}$$

When equation (5) is mapped into the space defined by the variables given by equations (8) to (11) and the new functions given by equations (12) to (14), one obtains the simplified differential given by

$$\left[2\,\frac{\partial}{\partial\eta_j} + \overline{\Sigma}_j\left(\eta_j,\xi_j\right)\right]\chi_j\left(\eta_j,\xi_j,\vec{x}_n,\vec{\Omega}\right) = g_j\left(\eta_j,\xi_j,\vec{x}_n,\vec{\Omega}\right) \tag{15}$$

which can be formally solved. Equation (15) may be integrated using the appropriate integrating factor, resulting in

$$\chi_j\left(\eta_j,\xi_j,\vec{x}_n,\vec{\Omega}\right) = \exp\left[-\frac{1}{2}\int_a^{\eta_j}\overline{\Sigma}_j\left(\eta',\xi_j\right)\,d\eta'\right]\chi_j\left(a,\xi_j,\vec{x}_n,\vec{\Omega}\right)$$

$$+ \frac{1}{2}\int_a^{\eta_j}\exp\left[-\frac{1}{2}\int_{\eta'}^{\eta_j}\overline{\Sigma}_j\left(\eta'',\xi_j\right)\,d\eta''\right]g_j\left(\eta',\xi_j,\vec{x}_n,\vec{\Omega}\right)\,d\eta' \tag{16}$$

where a is any real number. If the flux $\left(\text{that is, } \chi_j\left(\eta_j, \xi_j, \vec{x}_n, \vec{\Omega}\right)\right)$ is known at some point η_j given by the set of values $\eta_j = a$, ξ_j, $\vec{x}_n$, and $\vec{\Omega}$, then the flux at any other η_j may be found by using equation (16). The value a will be chosen later to always correspond to the boundary $\vec{\gamma}(s,t)$. Equation (16) may now be rewritten with the aid of equations (8) to (14) as

$$\overline{\phi}_j\left(\vec{x},\vec{\Omega},E\right) = \exp\left\{-\frac{1}{2}\int_a^{\rho-R_j(E)} \Sigma_j\left[R_j^{-1}\left(\frac{\xi_j - \eta'}{2}\right)\right] d\eta'\right\} \overline{\phi}_j\left[\left(\frac{\xi_j + a}{2}\right)\vec{\Omega} + \vec{x}_n, \vec{\Omega}, R_j^{-1}\left(\frac{\xi_j - a}{2}\right)\right]$$

$$+ \frac{1}{2}\int_a^{\rho-R_j(E)} \exp\left\{\frac{1}{2}\int_{\rho-R_j(E)}^{\eta''} \Sigma_j\left[R_j^{-1}\left(\frac{\xi_j - \eta'}{2}\right)\right] d\eta'\right\}$$

$$\times \overline{G}_j\left[\left(\frac{\xi_j + \eta''}{2}\right)\vec{\Omega} + \vec{x}_n, \vec{\Omega}, R_j^{-1}\left(\frac{\xi_j - \eta''}{2}\right)\right] d\eta'' \tag{17}$$

The value a will now be chosen such that the second factor of the first term on the right-hand side of equation (17) corresponds to the value at the boundary. Hence, a is chosen such that

$$\frac{\xi_j + a}{2}\vec{\Omega} + \vec{x}_n = \vec{\Gamma}_{\Omega,x} \tag{18}$$

The boundary point is shown in figure 1. The corresponding value of a is given by

$$a = 2\vec{\Omega} \cdot \vec{\Gamma}_{\Omega,x} - \xi_j = 2\vec{\Omega} \cdot \vec{\Gamma}_{\Omega,x} - \rho - R_j(E) \tag{19}$$

Using in equation (17) the variable transformations given by

$$E' = R_j^{-1}\left[\frac{\rho + R_j(E) - \eta'}{2}\right] \tag{20}$$

and

$$E'' = R_j^{-1}\left[\frac{\rho + R_j(E) - \eta''}{2}\right] \tag{21}$$

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so that

$$dE' = -\frac{S_j(E')}{2A_j} \, d\eta'$$ (22)

and

$$dE'' = -\frac{S_j(E'')}{2A_j} \, d\eta''$$ (23)

results in

$$\overline{\phi}_j\left(\vec{x},\vec{\Omega},E\right) = \exp\left[-\int_E^{R_j^{-1}\left[R_j(E)-d+\rho\right]} \frac{A_j\Sigma_j(E') \, dE'}{S_j(E')}\right]\overline{\phi}_j\left\{\vec{\Gamma}_{\Omega,x},\vec{\Omega},R_j^{-1}\left[R_j(E) - d + \rho\right]\right\}$$

$$+ \int_E^{R_j^{-1}\left[R_j(E)-d+\rho\right]} \exp\left[-\int_E^{E''} \frac{A_j\Sigma_j(E') \, dE'}{S_j(E')}\right]$$

$$\times \overline{G}_j\left\{\left[\left[\rho + R_j(E) - R_j(E'')\right]\vec{\Omega} + \vec{x}_n,\vec{\Omega},E''\right\}\frac{A_j \, dE''}{S_j(E'')}\right.$$ (24)

where

$$d = \vec{\Omega} \cdot \vec{\Gamma}_{\Omega,x}$$ (25)

Defining the total nuclear survival probability as

$$P_j(E) = \exp\left[-A_j \int_0^E \frac{\Sigma_j(E') \, dE'}{S_j(E')}\right]$$ (26)

results in

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$$\overline{\phi}_j\left(\overline{x},\vec{\Omega},E\right) = \frac{P_j\left\{R_j^{-1}\left[\rho - d + R_j(E)\right]\right\}}{P_j(E)} \, \overline{\phi}_j\left\{\overline{\Gamma}_{\Omega,x}, \vec{\Omega}, R_j^{-1}\left[\rho - d + R_j(E)\right]\right\}$$

$$+ \int_E^{R_j^{-1}\left[\rho - d + R_j(E)\right]} \frac{P_j(E')}{P_j(E)} \, \overline{G}_j\left\{\overline{x} + \left[R_j(E) - R_j(E')\right]\vec{\Omega}, \vec{\Omega}, E'\right\} \frac{A_j \, dE'}{S_j(E')} \tag{27}$$

Equation (27) can be further reduced using equations (6) and (7) to

$$\phi_j\left(\overline{x},\vec{\Omega},E\right) = \frac{S_j\left(E_\gamma\right) P_j\left(E_\gamma\right)}{S_j(E) P_j(E)} \, \phi_j\left(\overline{\Gamma}_{\Omega,x}, \vec{\Omega}, E_\gamma\right)$$

$$+ \int_E^{E_\gamma} \frac{A_j P_j(E')}{S_j(E) P_j(E)} \, G_j\left\{\overline{x} + \left[R_j(E) - R_j(E')\right]\vec{\Omega}, \vec{\Omega}, E'\right\} \, dE' \tag{28}$$

where

$$E_\gamma = R_j^{-1}\left[\rho - d + R_j(E)\right] \tag{29}$$

Using the definition of $G_j\left(\overline{x},\vec{\Omega},E\right)$ (eq. (4)) in equation (28) results in

$$\phi_j\left(\overline{x},\vec{\Omega},E\right) = \frac{S_j\left(E_\gamma\right) P_j\left(E_\gamma\right)}{S_j(E) P_j(E)} \, \phi_j\left(\overline{\Gamma}_{\Omega,x}, \vec{\Omega}, E_\gamma\right)$$

$$+ \sum_k \int_E^{E_\gamma} dE' \, \frac{A_j P_j(E')}{S_j(E) P_j(E)} \int_{E'}^\infty dE'' \int d\vec{\Omega}' r_{jk}\left(E',E'',\vec{\Omega},\vec{\Omega}'\right)$$

$$\times \, \phi_k\left\{\overline{x} + \left[R_j(E) - R_j(E')\right]\vec{\Omega}, \vec{\Omega}', E''\right\} \tag{30}$$

which is the integral equation of heavy-ion transport theory. Techniques for the approximate solution of equation (30), or equivalently equation (1), with the boundary condition (eq. (2)) are considered next.

INTERACTION PARAMETERS

The parameter appearing in equation (1) relating to interaction of ions with orbital electrons is the energy loss per unit path length, denoted by $S_j(E)$. For the present, fluctuations about the mean will be ignored and the simplified approximation (see refs. 16 to 18 for discussion)

$$S_j(E) = \frac{4\pi e^4 z_j^2}{m_e v^2} N_m B \qquad (31)$$

will be used, where

$$B = z_m \left[\ln\left(\frac{2m_e v^2}{I}\right) + \psi(1) - \mathrm{Re}\,\psi\left(1 + \frac{iz_j e^2}{\hbar v}\right) \right] \qquad (32)$$

$$\psi(x) = \frac{1}{\Gamma(x)} \frac{d}{dx} \Gamma(x) \qquad (33)$$

N_m is the atom density of the material, z_m is the material atomic number, I is the material adjusted ionization potential, m_e is the electron mass, e is the electron charge, $\hbar$ is Planck's constant, v is the ion velocity, and z_j is the ion atomic number. Equations (31) to (33) apply at large ion velocities. As the ion slows, it tends to capture orbital electrons, which effectively reduces the ion charge. The effective ion charge z_j^* will be taken as (ref. 16)

$$z_j^* = z_j \left[1 - \exp\left(-125\, v \Big/ c z_j^{2/3}\right) \right] \qquad (34)$$

where v is the ion speed and c is the speed of light. In addition to orbital electron capture, the nuclear elastic scattering also becomes important at very low energies. If the ion speed is sufficiently large, it is clear from equations (31) through (33) that

$$S_j(E) = \left(\frac{z_j^*}{z_p^*}\right)^2 S_p(E) \qquad (35)$$

where $S_p(E)$ is the proton stopping power and z_p^* is the effective proton charge. Empirically, it is found that equation (35) is reasonably accurate even at low ion speeds. Expressions (31) to (33) fail at low energies but the empirical expression (for energy loss in water)

$$S_p(E) \approx E^{0.303}(2517 - 6283E) \tag{36}$$

and equation (35) may be used for energy E less than 243.8 keV/amu.

The parameters in equations (1) and (30) which are least known are those associated with the nuclear attenuation and fragmentation. If the elastic scattering of heavy ions is ignored to a first approximation, then $\Sigma_j(E)$ is the ion macroscopic absorption cross section for the transport medium. The microscopic cross sections from which $\Sigma_j(E)$ is determined are presented in reference 10.

The fragmentation of the ion and target nuclei is represented by the quantities $r_{jk}(E,E',\vec{\Omega},\vec{\Omega}')$ which are composed of three functions as follows:

$$r_{jk}(E,E',\vec{\Omega},\vec{\Omega}') = \Sigma_k(E')\nu_{jk}(E')f_{jk}(E,E',\vec{\Omega},\vec{\Omega}') \tag{37}$$

where $\nu_{jk}(E')$ is the multiplicity of type j ions being produced by a collision of a type k ion of energy E' and $f_{jk}(E,E',\vec{\Omega},\vec{\Omega}')$ is the probability density distribution for producing type j ions of energy E into direction $\vec{\Omega}$ from the collision of a type k ion with energy E' moving in direction $\vec{\Omega}'$. For an unpolarized source of ions and unpolarized targets, the energy-angle distribution of reaction products may be taken as a function of the energies and cosine of the production angle with respect to the incident beam direction. The secondary multiplicities $\nu_{jk}(E)$ and secondary energy-angle distributions are the major unknowns in ion transport theory.

Until recently, information on the multiplicity $\nu_{jk}(E)$ was obtained through experiments with galactic cosmic rays as an ion source and the fragmentation of the ions on target nuclei was observed in nuclear emulsion (ref. 19). Such data are mainly limited by not knowing the identity of the initial or secondary ions precisely and by relatively low counting rates of each ion type. Recent heavy-ion acceleration by machine makes it possible to reduce the uncertainty since large count rates are possible with known ion types. In addition, the target nuclei in accelerator experiments can conveniently be other than nuclear emulsion, and accurate detector techniques with modern electronic processing are greatly improving the experimental data base. In addition, the accelerator experiments

are providing information on the spectral distribution $f_{jk}(E,E',\vec{\Omega},\vec{\Omega}')$ which has not before been available (ref. 20).

The spectral distribution function is found to consist of two terms which describe the fragmentation of the projectile and the fragmentation of the struck nucleus as follows (refs. 21 and 22):

$$r_{jk}(E,E',\vec{\Omega},\vec{\Omega}') = \Sigma_k(E')\left[\nu_{jk}^P(E')f_{jk}^P(E,E',\vec{\Omega},\vec{\Omega}') + \nu_{jk}^T(E')f_{jk}^T(E,E',\vec{\Omega},\vec{\Omega}')\right] \tag{38}$$

where ν_{jk}^P and f_{jk}^P depend only weakly on the target and ν_{jk}^T and f_{jk}^T depend only weakly on the projectile. Whereas the average secondary velocities associated with f^P are nearly equal to the projectile velocity, the average velocities associated with f^T are near zero. Experimentally (refs. 20 to 22), it is observed that

$$f_{jk}^P(E,E',\vec{\Omega},\vec{\Omega}') \approx \left[\frac{m}{2\pi\left(\sigma_{jk}\right)^2}\right]^{3/2}\sqrt{2E}\,\exp\left[-\frac{\left(\vec{p}-\vec{p}'\right)^2}{2\left(\sigma_{jk}^T\right)^2}\right]$$

$$\approx \left[\frac{m}{2\pi\left(\sigma_{jk}\right)^2}\right]^{3/2}\sqrt{2E}\,\exp\left[-\frac{\left(\sqrt{2mE}\,\vec{\Omega}-\sqrt{2mE'}\,\vec{\Omega}'\right)^2}{2\left(\sigma_{jk}^T\right)^2}\right] \tag{39}$$

$\left(\text{where }\vec{p}\text{ and }\vec{p}'\text{ are the momenta per unit mass of }j\text{ and }k\text{ ions, respectively}\right)$ and

$$f_{jk}^T(E,E',\vec{\Omega},\vec{\Omega}') \approx \left[\frac{m}{2\pi\left(\sigma_{jk}^T\right)^2}\right]^{3/2}\sqrt{2E}\,\exp\left[-\frac{\vec{p}^2}{2\left(\sigma_{jk}^T\right)^2}\right] \tag{40}$$

where σ_{jk}^P and σ_{jk}^T are related to the rms momentum spread of secondary products. These parameters depend only on the fragmenting nucleus. It was first suggested by Feshbach and Huang (ref. 7) that the parameters σ_{jk}^P and σ_{jk}^T depend on the average square momentum of the nuclear fragments as allowed by Fermi motion. A precise formulation of these ideas in terms of a statistical model was obtained by Goldhaber (ref. 8).

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APPROXIMATION PROCEDURES

Neglect of Target Fragmentation

Employing equations (37) to (40) in the evaluation of $G_j(\vec{x},\vec{\Omega},E)$ of equation (4) results in

$$G_j(\vec{x},\vec{\Omega},E) = \sum_k \int dE' \, d\vec{\Omega}' \, \Sigma_k(E') \, \phi_k(\vec{x},\vec{\Omega}',\vec{E}') \left[\nu_{jk}^P(E') \, f_{jk}^P(E,E',\vec{\Omega},\vec{\Omega}') + \nu_{jk}^T f_{jk}^T(E,E',\vec{\Omega},\vec{\Omega}') \right]$$

$$\equiv G_j^P(\vec{x},\vec{\Omega},E) + G_j^T(\vec{x},\vec{\Omega},E) \tag{41}$$

where, as before, the superscripts P and T refer to fragmentation of the projectile and target, respectively. The target term is seen to be

$$G_j^T(\vec{x},\vec{\Omega},E) = \sum_k \left[\frac{m}{2\pi\left(\sigma_{jk}^T\right)^2} \right]^{3/2} \sqrt{2E} \, \exp\left[-mE \Big/ \left(\sigma_{jk}^T\right)^2 \right] \int d\vec{\Omega}' \int_E^\infty dE' \, \nu_{jk}^T(E') \, \Sigma_k(E') \, \phi_k(\vec{x},\vec{\Omega}',E') \tag{42}$$

which is negligibly small for

$$E \gg \left(\sigma_{jk}^T\right)^2 \Big/ m \tag{43}$$

Thus, for calculating the flux at high energy,

$$G_j(\vec{x},\vec{\Omega},E) \approx G_j^P(\vec{x},\vec{\Omega},E) \tag{44}$$

Space Radiations

A convenient property of space radiations is that they are nearly isotropic. This fact, coupled with the forward peaked spectral distribution, leads to substantial reductions in the source term as follows:

$$G_j^P(\vec{x},\vec{\Omega},E) \approx \sum_k \int dE' \, d\vec{\Omega}' \, \Sigma_k(E') \, \nu_{jk}^P(E') \left[\frac{m}{2\pi\left(\sigma_{jk}^P\right)^2} \right]^{3/2} \sqrt{2E'}$$

$$\times \exp\left[-\frac{\left(\sqrt{2mE}\,\vec{\Omega} - \sqrt{2mE'}\,\vec{\Omega}'\right)^2}{2\left(\sigma_{jk}^P\right)^2} \right] \phi_k(\vec{x},\vec{\Omega}',E') \tag{45}$$

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Assuming that $\phi_k(\vec{x}, \vec{\Omega}', E')$ is a slowly varying function of $\vec{\Omega}'$, one may seek an expansion about the sharply peaked maximum of the exponential function. Such an expansion is made by letting

$$\vec{\Omega}' = \vec{\Omega} + (\cos\theta - 1)\vec{\Omega} + \sin\theta \; \vec{e}_\phi \tag{46}$$

where

$$\cos\theta = \vec{\Omega} \cdot \vec{\Omega}' \tag{47}$$

and

$$\vec{e}_\phi = \vec{\Omega} \times \vec{\Omega}' \big/ \left| \vec{\Omega} \times \vec{\Omega}' \right| \tag{48}$$

with which the flux may be expanded as

$$\phi_k(\vec{x}, \vec{\Omega}', E') = \phi_k(\vec{x}, \vec{\Omega}, E') + \left[\frac{\partial}{\partial\vec{\Omega}} \phi_k(\vec{x}, \vec{\Omega}, E') \right] \cdot \left[(\cos\theta - 1)\vec{\Omega} + \sin\theta \; \vec{e}_\phi \right] + \ldots \tag{49}$$

Substituting equation (49) into equation (45) and simplifying results in

$$G_j^P(\vec{x}, \vec{\Omega}, E) \approx \sum_k \int dE' \; \Sigma_k(E') \, \nu_{jk}^P(E') \left[\frac{m}{2\pi \left(\sigma_{jk}^P \right)^2} \right]^{3/2} \frac{\sqrt{2}}{\sqrt{E'}} \exp\left[-\frac{\left(\sqrt{2mE} - \sqrt{2mE'} \right)^2}{2 \left(\sigma_{jk}^P \right)^2} \right]$$

$$\times \left\{ \phi_k(\vec{x}, \vec{\Omega}, E') - \left[\vec{\Omega} \cdot \frac{\partial}{\partial\vec{\Omega}} \phi_k(\vec{x}, \vec{\Omega}, E') \right] \left[\frac{\left(\sigma_{jk}^P \right)^2}{2m\sqrt{EE'}} \right] + \ldots \right\} \tag{50}$$

The leading term of equation (50) is clearly a good approximation to the source term whenever

$$\frac{2mE}{\left(\sigma_{jk}^P \right)^2} \gg \frac{\vec{\Omega} \cdot \frac{\partial}{\partial\vec{\Omega}} \phi_k(\vec{x}, \vec{\Omega}, E')}{\phi_k(\vec{x}, \vec{\Omega}, E')} \tag{51}$$

Note that the leading term is equivalent to assuming that secondary ions are produced only in the direction of motion of the primary ions. In the case of space radiations which are nearly isotropic, relation (51) is easily satisfied and neglect of higher-order terms

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in equation (50) results in the usual straightahead approximation. If the radiation is highly anisotropic, then relation (51) is not likely to apply. Such behavior was discovered empirically by Alsmiller et al. (refs. 23 and 24) for the case of proton transport.

Velocity Conserving Interaction

It has been customary in cosmic ion transport studies (ref. 1) to assume that the fragment velocities are equal to the fragmenting ion velocity prior to collision. Derived below is the order of approximation resulting from such an assumption. If it is assumed that the projectile energy E' is equal to the secondary energy plus a positive quantity ϵ

$$E' = E + \epsilon \tag{52}$$

and that ϵ will contribute to equation (50) only over a small range above zero energy, substituting equation (52) into equation (50) and expanding the integrand results in

$$G_j^P\left(\vec{x},\vec{\Omega},E\right) = \sum_k \Sigma_k(E)\, \nu_{jk}^P(E) \left\{ \phi_k\left(\vec{x},\vec{\Omega},E\right)\left[1 - \sqrt{\frac{\left(\sigma_{jk}^P\right)^2}{\pi mE}}\right] \right.$$
$$\left. + \left[E\frac{\partial}{\partial E}\phi_k\left(\vec{x},\vec{\Omega},E\right)\right]\sqrt{\frac{\left(\sigma_{jk}^P\right)^2}{\pi mE}} - \left[\vec{\Omega}\cdot\frac{\partial}{\partial\vec{\Omega}}\phi_k\left(\vec{x},\vec{\Omega},E\right)\right]\frac{\left(\sigma_{jk}^P\right)^2}{2mE} + \ldots \right\} \tag{53}$$

Since $\sqrt{\dfrac{\left(\sigma_{jk}^P\right)^2}{mE}} \ll 1$ at those energies for which most nuclear reactions occur, it is clear that the assumption of velocity conservation is inferior to a straightahead approximation but may be adequate for space radiations where the variation of $\phi_k\left(\vec{x},\vec{\Omega},E\right)$ with energy is sufficiently smooth. That is,

$$E\frac{\partial}{\partial E}\phi_k\left(\vec{x},\vec{\Omega},E\right) \approx \phi_k\left(\vec{x},\vec{\Omega},E\right)$$

Decoupling of Target and Projectile Flux

Equation (1) with the use of equation (41) may be rewritten as

$$B_j\phi_j\left(\vec{x},\vec{\Omega},E\right) = \sum_k F_{jk}^T\,\phi_k\left(\vec{x},\vec{\Omega},E\right) + \sum_k F_{jk}^P\,\phi_k\left(\vec{x},\vec{\Omega},E\right) \tag{54}$$

where the differential operator is given by

$$B_j = \left[\vec{\Omega} \cdot \nabla - \frac{1}{A_j} \frac{\partial}{\partial E} S_j(E) + \Sigma_j(E) \right] \tag{55}$$

and the integral operator $\left(F_{jk} = F_{jk}^T + F_{jk}^P \right)$ is given by

$$F_{jk}\phi_k\left(\vec{x},\vec{\Omega},E\right) = \int dE' \, d\vec{\Omega}' \, r_{jk}\left(E,E',\vec{\Omega},\vec{\Omega}'\right) \phi_k\left(\vec{x},\vec{\Omega}',E'\right) \tag{56}$$

Defining the flux as a sum of two terms

$$\phi_j\left(\vec{x},\vec{\Omega},E\right) = \phi_j^T\left(\vec{x},\vec{\Omega},E\right) + \phi_j^P\left(\vec{x},\vec{\Omega},E\right) \tag{57}$$

allows the following separation:

$$B_j\phi_j^P\left(\vec{x},\vec{\Omega},E\right) = \sum_k F_{jk}^P\phi_k^P\left(\vec{x},\vec{\Omega},E\right) + \sum_k F_{jk}^P\phi_k^T\left(\vec{x},\vec{\Omega},E\right) \tag{58}$$

$$B_j\phi_j^T\left(\vec{x},\vec{\Omega},E\right) = \sum_k F_{jk}^T\phi_k^P\left(\vec{x},\vec{\Omega},E\right) + \sum_k F_{jk}^T\phi_k^T\left(\vec{x},\vec{\Omega},E\right) \tag{59}$$

As noted in connection with equations (42) through (44), the source term on the right-hand side of equation (59) is small at high energies and one may assume

$$\phi_j^T\left(\vec{x},\vec{\Omega},E\right) \approx 0 \tag{60}$$

for $E \gg \left(\sigma_{jk}^T\right)^2 \big/ m$. As a result of equation (60) and the fact that the ion range is small compared with its mean free path at low energy, one obtains

$$B_j\phi_j^P\left(\vec{x},\vec{\Omega},E\right) \approx \sum_k F_{jk}^P\phi_k^P\left(\vec{x},\vec{\Omega},E\right) \tag{61}$$

$$B_j\phi_j^T\left(\vec{x},\vec{\Omega},E\right) \approx \sum_k F_{jk}^T\phi_k^P\left(\vec{x},\vec{\Omega},E\right) \tag{62}$$

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The advantage of this separation is that once equation (61) is solved by whatever means necessary, then equation (62) can be solved in closed form. The solution of equation (62) is accomplished by noting that the inwardly directed flux ϕ_j^T must vanish on the boundary, so that

$$\phi_j^T\left(\vec{x},\vec{\Omega},E\right) \approx \sum_k \int_E^{E_\gamma} dE' \; \frac{A_j P_j(E')}{P_j(E)S_j(E)} \int dE'' \; d\vec{\Omega}' \, r_{jk}^T\left(E',E'',\vec{\Omega},\vec{\Omega}'\right)$$

$$\times \phi_k^P \left\{\vec{x} + \left[R_j(E) - R_j(E')\right]\vec{\Omega},\vec{\Omega}',E''\right\} \tag{63}$$

where E_γ is given by equation (29).

Using equations (38) and (40) in equation (63) yields

$$\phi_j^T\left(\vec{x},\vec{\Omega},E\right) \approx \int_E^{E_\gamma} dE' \; \frac{A_j P_j(E')}{P_j(E)S_j(E)} \left[\frac{m}{2\pi\left(\sigma_{jk}^T\right)^2}\right]^{3/2} \sqrt{2E'} \; e^{-mE'\Big/\left(\sigma_{jk}^T\right)^2}$$

$$\times \zeta_j \left\{\vec{x} + \left[R_j(E) - R_j(E')\right]\vec{\Omega}\right\} \tag{64}$$

where

$$\zeta_j\left(\vec{x}\right) = \sum_k \int dE' \; d\vec{\Omega}' \, \Sigma_k(E') \, \nu_{jk}^T(E') \, \phi_k^P\left(\vec{x},\vec{\Omega}',E'\right) \tag{65}$$

and σ_{jk}^T has been assumed to be a slowly varying function of projectile type k and projectile energy E. If the range of secondary type j ions is small compared with their mean free path lengths and the mean free paths of the fragmenting parent ions ℓ_k, that is,

$$R_j\left[\left(\sigma_{jk}^T\right)^2\Big/m\right] \ll \ell_k \tag{66}$$

then the integral of equation (64) may be simplified as

$$\phi_j^T\left(\vec{x},\vec{\Omega},E\right) \approx \frac{A_j}{S_j(E)} \zeta_j\left(\vec{x}\right) \int_E^{E_\gamma} \left[\frac{m}{2\pi\left(\sigma_{jk}^T\right)^2}\right]^{3/2} \sqrt{2E'} \; e^{-mE'\Big/\left(\sigma_{jk}^T\right)^2} dE' \tag{67}$$

which may be reduced into terms of known functions. Thus,

$$\phi_j^T\left(\vec{x},\vec{\Omega},E\right) \approx \frac{A_j}{S_j(E)}\,\zeta_j\left(\vec{x}\right)\frac{1}{2\pi\sqrt{\pi}}\left\{\Gamma\left[\frac{3}{2},\frac{mE}{\left(\sigma_{jk}^T\right)^2}\right] - \Gamma\left[\frac{3}{2},\frac{mE_\gamma}{\left(\sigma_{jk}^T\right)^2}\right]\right\} \tag{68}$$

in terms of the incomplete gamma function. It may also be shown that equation (68) is equivalent to

$$\phi_j^T\left(\vec{x},\vec{\Omega},E\right) \approx \frac{A_j}{S_j(E)}\,\zeta_j\left(\vec{x}\right)\frac{1}{2\pi}\left\{\frac{1}{2}\,\text{erfc}\left[\sqrt{\frac{mE}{\left(\sigma_{jk}^T\right)^2}}\right] - \frac{1}{2}\,\text{erfc}\left[\sqrt{\frac{mE_\gamma}{\left(\sigma_{jk}^T\right)^2}}\right]\right.$$

$$\left. + \sqrt{\frac{mE}{\pi\left(\sigma_{jk}^T\right)^2}}\,e^{-mE\Big/\left(\sigma_{jk}^T\right)^2} - \sqrt{\frac{mE_\gamma}{\pi\left(\sigma_{jk}^T\right)^2}}\,e^{-mE_\gamma\Big/\left(\sigma_{jk}^T\right)^2}\right\} \tag{69}$$

At points sufficiently removed from the boundary such that

$$R_j^{-1}(\rho - d) \gg \left(\sigma_{jk}^T\right)^2\Big/m \tag{70}$$

equation (69) may be reduced to

$$\phi_j^T\left(\vec{x},\vec{\Omega},E\right) \approx \frac{A_j}{S_j(E)}\,\zeta_j\left(\vec{x}\right)\frac{1}{2\pi}\left\{\frac{1}{2}\,\text{erfc}\left[\sqrt{\frac{mE}{\left(\sigma_{jk}^T\right)^2}}\right] + \sqrt{\frac{mE}{\pi\left(\sigma_{jk}^T\right)^2}}\,e^{-mE\Big/\left(\sigma_{jk}^T\right)^2}\right\} \tag{71}$$

The solution of equation (61) will now be further examined.

Back-Substitution and Perturbation Theory

One approach to the solution of equation (61) results from the fact that the multiply charged ions tend to be destroyed in nuclear reactions. Thus,

$$F_{jk}^P \equiv 0 \qquad\qquad (j \geq k) \tag{72}$$

This means that there is a maximum j such that

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$$B_J \phi_J^P(\vec{x}, \vec{\Omega}, E) = 0 \tag{73}$$

where J is the largest j. Furthermore,

$$B_{J-1} \phi_{J-1}^P(\vec{x}, \vec{\Omega}, E) = F_{J-1,J}^P \phi_J^P(\vec{x}, \vec{\Omega}, E) \tag{74}$$

and, in general,

$$B_{J-N} \phi_{J-N}^P(\vec{x}, \vec{\Omega}, E) = \sum_{k=1}^{N-1} F_{J-N,J-k}^P \phi_{J-k}^P(\vec{x}, \vec{\Omega}, E) \tag{75}$$

for $N < J - 1$. Note that equations (73) to (75) constitute solvable problems. The singly charged ions satisfy

$$B_1 \phi_1^P(\vec{x}, \vec{\Omega}, E) = F_{1,1}^P \phi_1^P(\vec{x}, \vec{\Omega}, E) + \sum_{k=2}^{J} F_{1,k}^P \phi_k^P(\vec{x}, \vec{\Omega}, E) \tag{76}$$

which, unlike equations (73) to (75), is an integral-differential equation, which is difficult to solve directly. Equation (76) is solvable by perturbation theory and the resultant series is known to converge rapidly for intermediate and low energies (ref. 11). It is to be noted that equations (73) to (75) are also obtained from perturbation theory as applied to equation (61) at the outset. Thus, the perturbation series is expected to converge after the first J plus a few terms.

When J is large, the number of terms entering the summations in equations (75) and (76) may lead to a lengthy computational problem. An estimate of the number of terms required to adequately approximate the solution of equation (75) would be useful before a commitment to the development of computer programs to evaluate the series is made. For this purpose, a study of a simplified but realistic model is undertaken to determine the rate of convergence of the perturbation series.

MODEL CALCULATION

At sufficiently high energies, the energy loss can be neglected over many mean free paths of the incident ion. Assuming the straightahead approximation is valid and that all secondary fragments have the same velocity as the fragmenting parent nucleus leads to

a particularly simple one-dimensional form of the theory. Namely, equation (1) becomes

$$\left(\frac{\partial}{\partial x} + \Sigma_j\right)\phi_j(x) = \sum_k \Sigma_k \nu_{jk}^P \phi_k(x) \tag{77}$$

which may likewise be written as

$$\phi_j(x) = e^{-\Sigma_j x}\phi_j(0) + \int_0^x e^{\Sigma_j(x'-x)} \sum_k \Sigma_k \nu_{jk}^P \phi_k(x')\, dx' \tag{78}$$

which is equivalent to equation (30). For the present example, a simple form for Σ_k and ν_{jk}^P which is reasonably realistic is assumed. Namely, we take

$$\Sigma_k = \Sigma_0 k^{2/3} \tag{79}$$

and

$$\nu_{jk}^P = \frac{2}{k-1}\, u(k-j) \tag{80}$$

where j and k are to be interpreted as ion charge numbers and u is the unit step function; it is seen that equation (80) conserves charge in the interaction. Implicit in equations (79) and (80) is the neglect of target fragmentation products.

Equation (78) was solved numerically using successive interations and numerical quadrature. The zeroth-order approximation was taken as

$$\phi_j^{(0)}(x) = e^{-\Sigma_j x}\phi_j(0) \tag{81}$$

and the higher-order corrections were added by substitution into the right-hand side of equation (78), giving

$$\phi_j^{(i+1)}(x) = e^{-\Sigma_j x}\phi_j(0) + \sum_k \Sigma_k \nu_{jk}^P \int_0^x e^{\Sigma_j(x'-x)} \phi_k^{(i)}(x')\, dx' \tag{82}$$

for $i = 0, 1, 2, \ldots$. The Σ_0 parameter in equation (79) was chosen to correspond to air and the boundary condition was taken as

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$$\phi_j(0) = \delta_{j,25} \tag{83}$$

corresponding to an iron group nucleus incident on the Earth's atmosphere. The iteration procedure converged over the first 60 g/cm^2 in six iterations and numerical errors were held to within 10 percent. Thus, it appears that perturbation theory may well result in a practical calculation procedure for heavy-ion transport for most applications.

The integrated ion flux as calculated with the iteration procedure indicated in equation (82) is shown in figure 2, along with the integrated ion flux as calculated with only the first-order correction (that is, $i = 0$ in eq. (82) only). It is seen that the first-order result is far from accurate over most of the regions of interest. Although first-order theory is inadequate in this respect, the predicted average charge of the beam as it passes through the air is no worse than a factor of two off, as shown in figure 3. Although the average charge is approximately correct, 96 percent of the initial charge of 25 is contained in higher-order terms at 60 g/cm^2. The importance of higher-order terms is shown again in connection with the calculation of secondary particle dose in figure 4. Clearly, doses calculated on the basis of first-order theory contain large errors for depths beyond several g/cm^2 of material.

The dose contribution from various charge components is shown in figure 5 at several depths. Also shown for comparison are the results of first-order theory for the two lowest values of depth. Most conspicuous is that the maximum contribution comes from a broad range of charges above $z = 3$. This is even true at rather great depths such as the 59.2 g/cm^2 curve in the figure, which represents nearly four mean free path lengths of the primary ion beam.

The results in figure 5 are of importance in the evaluation of the biological effects since it is well known that heavy ions can bring about biological effects not observed with any other known types of radiation. The fact that secondary ions formed from the fragmentation of a single larger ion have greater penetrating power and may be even more damaging biologically as a result of saturation effects points out the need for a careful evaluation of transport effects on biological systems shielded from high-energy heavy-ion radiation. Such an evaluation would also be important with respect to evaluation of doses in connection with radiotherapy (especially in surrounding healthy tissues).

Aside from the damaging effects of secondary projectile fragments, the nuclear stars formed by fragmenting target nuclei will sometimes be of major importance. In this connection, the collision density is of importance as shown in figure 6. Again it is seen that a first-order calculation does not produce the required accuracy for most applications.

CONCLUDING REMARKS

The fundamental equations of heavy-ion transport are presented both as a set of integral/partial-differential equations and as a coupled set of inhomogeneous integral equations. The basic interaction parameters are discussed and simple approximations based on experimental observations are given. On the basis of these interaction parameters, simplifications of the fundamental transport equations are discussed. An iterative method is proposed to solve the inhomogeneous integral equations for which rapid convergence is obtained in a transport model which neglects ionization energy loss, assumes forward secondary particle production, and assumes the secondary particle velocity is equal to the fragmenting ions velocity. Although a first-order perturbation theory is generally insufficient to represent the transport process, six correction terms provide sufficient accuracy for the iron group ions for most depth ranges of interest (≤ 60 g/cm^2). It is found in these model calculations that the secondary multiply charged ions can penetrate well beyond the depths obtainable by the primary ion. This fact will be most important in connection with space and high-altitude aircraft shielding and radiotherapy.

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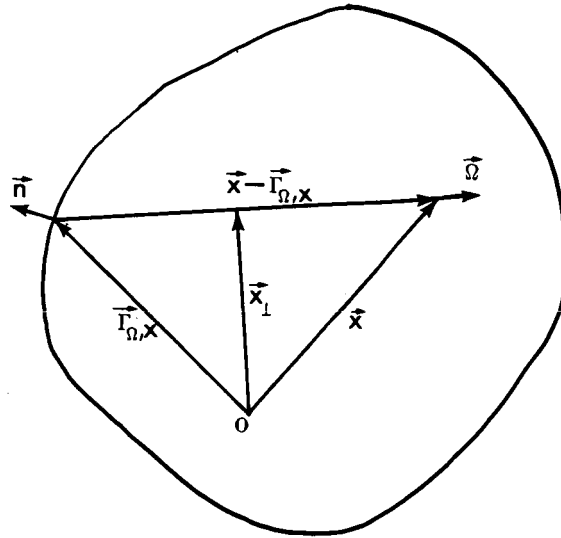
Figure 1.- Relation of boundary and vector quantities required
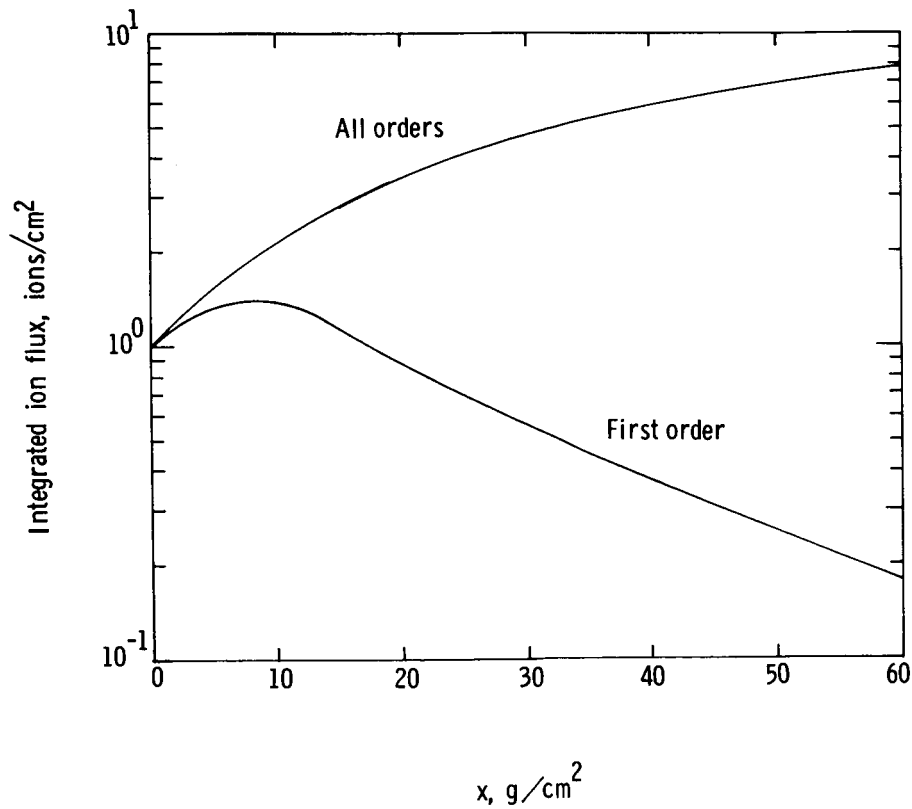for evaluation of ion fields.

Figure 2.- Integrated ion flux as result of normally incident iron group
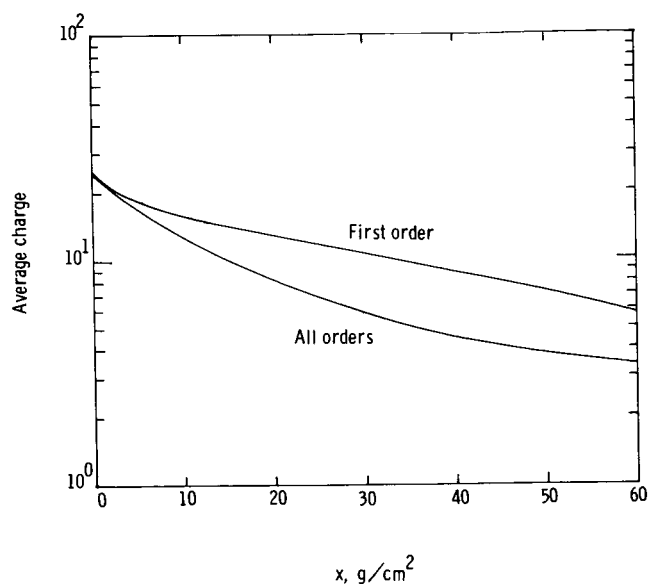ion flux on top of Earth's atmosphere.

Figure 3.- Average charge of ions produced in Earth's atmosphere by normally incident high-energy iron group ion integrated flux.
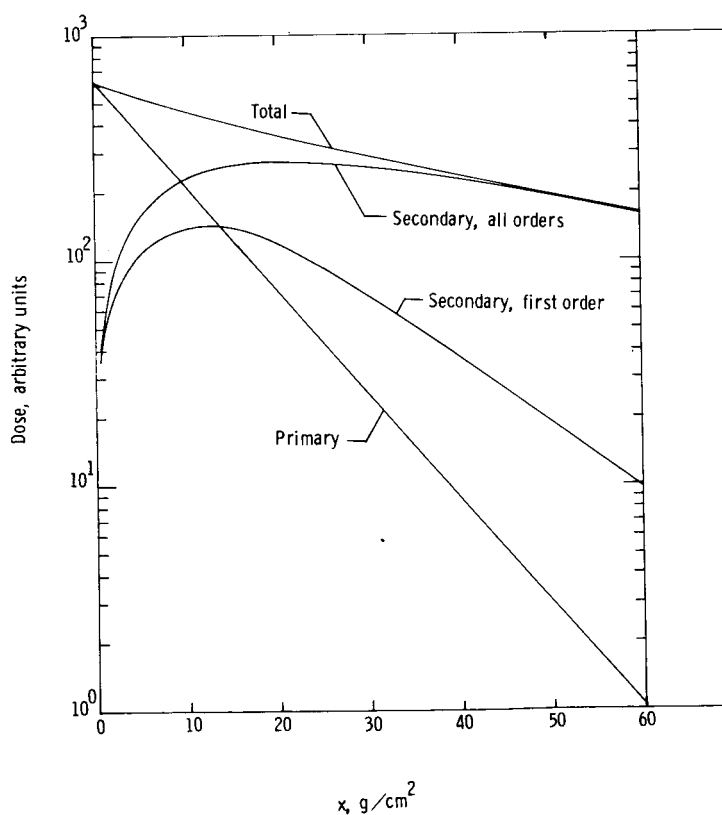

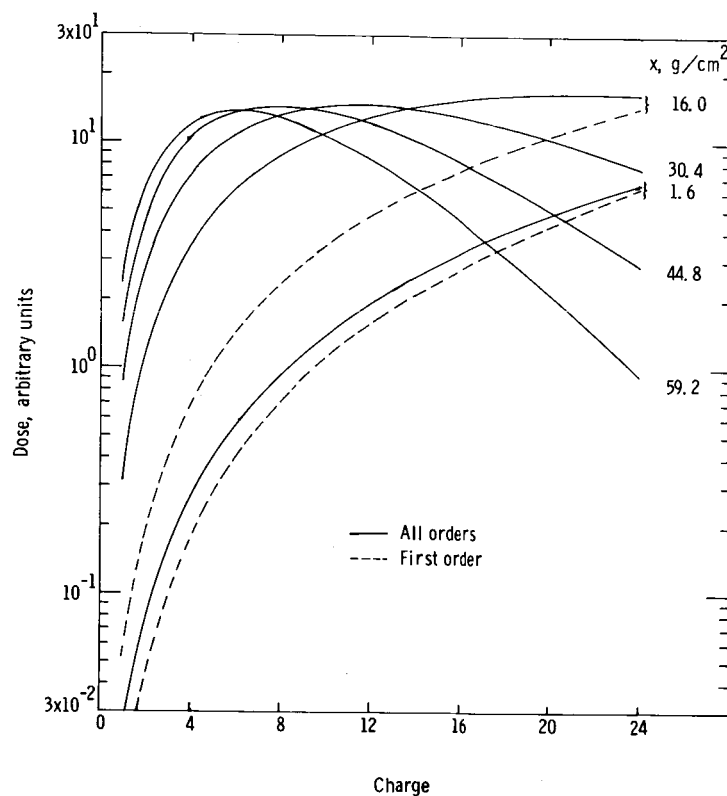Figure 4.- Dose in Earth's atmosphere due to normally incident iron group integrated flux ($1/cm^2$) of high energy.

Figure 5.- Dose contribution from various ion types in Earth's atmosphere due to normally incident high-energy iron group ion integrated flux $(1/cm^2)$.
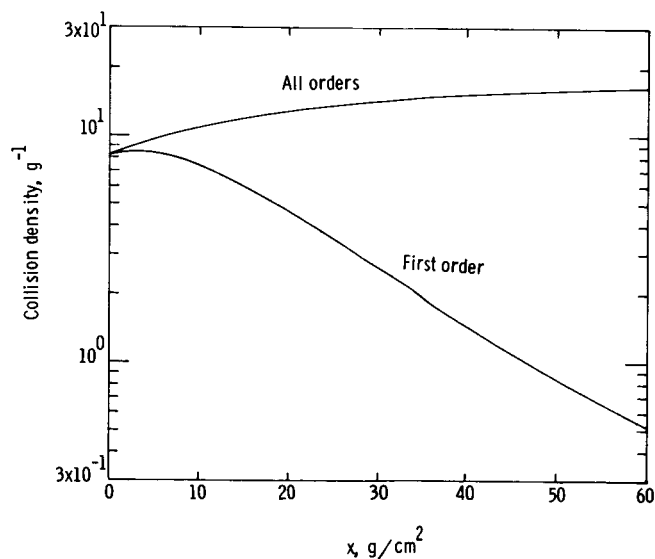

Figure 6.- Density of nuclear reactions with air nuclei produced by normally incident iron group ion integrated flux $(1/cm^2)$ and all secondary fragments.