

Neutron Transport Models and Methods for HZETRN and Coupling to Low Energy Light Ion Transport

T. C. Slaba and J. H. Heinbockel
Old Dominion University

S. R. Blattnig
NASA Langley Research Center

Copyright © 2008 SAE International

ABSTRACT

Exposure estimates inside space vehicles, surface habitats, and high altitude aircraft exposed to space radiation are highly influenced by secondary neutron production. The deterministic transport code HZETRN has been identified as a reliable and efficient tool for such studies, but improvements to the underlying transport models and numerical methods are still necessary. In this paper, the forward-backward (FB) and directionally coupled forward-backward (DC) neutron transport models are derived, numerical methods for the FB model are reviewed, and a computationally efficient numerical solution is presented for the DC model. Both models are compared to the Monte Carlo codes HETC-HEDS and FLUKA, and the DC model is shown to agree closely with the Monte Carlo results. Finally, it is found in the development of either model that the decoupling of low energy neutrons from the light ion ($A \leq 4$) transport procedure adversely affects low energy light ion fluence spectra and exposure quantities. A first order correction is presented to resolve the problem, and it is shown to be both accurate and efficient.

INTRODUCTION

Radiation exposure guidelines are a primary concern for the design of high altitude aircraft, personal shielding, spacecraft, instrumentation, and mission planning. Consequently, there is significant interest in developing computational tools that allow shield analyses not only in simplified geometries, but in more complex final design models as well.¹ The deterministic transport code HZETRN²⁻⁶ developed at NASA Langley Research Center has emerged in recent years as a reliable and efficient tool for such studies. It has shown reasonable accuracy in deep space galactic cosmic ray (GCR), solar particle event (SPE), and low earth orbit (LEO) simulations when compared to either Monte Carlo results or experimental data.⁷ However, such verification and validation has revealed a deficiency in the low energy

neutron transport procedure.⁸ HZETRN utilizes the straight-ahead approximation in which all fragments are assumed to propagate in the same direction as the projectile. The assumption is accurate for high energy charged particles but breaks down for low energy neutrons which are produced nearly isotropically.⁹ This is significant for heavily shielded space vehicles, surface habitats, and high altitude aircraft where secondary neutron production is important in exposure calculations.¹⁰

Several neutron transport models have been developed for HZETRN, with recent efforts focused on identifying an optimal bi-directional neutron transport model and solution method. The terms model and method are used extensively throughout this paper; model is used to refer to the set of governing transport equations, while method is used to refer to the analytic or numerical techniques used to solve a model. Heinbockel *et al.*¹¹ and Cloudsley *et al.*^{12,13} developed the forward-backward (FB) neutron transport model. It assumes that low energy neutrons can be split into forward and backward components, and multiple reflections from forward to backward (or vice versa) can be ignored. Feldman¹⁴ expanded on the work of Heinbockel and Cloudsley by developing the directionally coupled forward-backward neutron transport model. It also assumes that low energy neutrons can be split into forward and backward components, but multiple reflections are accounted for in the governing transport equations. The numerical methods used for each model were drastically different as well.

Heinbockel *et al.*¹¹ and Cloudsley *et al.*^{12,13} used a multigroup method for solving the FB model. Multigroup methods have a long history in nuclear reactor theory and assume that fluences or cross sections are constant over small regions, or groups, of the energy spectrum.¹⁵ Marchuk *et al.*¹⁵ gives a more general description of this method. Feldman¹⁴ used a collocation technique along with first order finite differencing for the DC model. Collocation and finite differencing methods use

polynomial expansions or approximations to transform a differential equation into a system of linear equations.¹⁶ In this case, the system was sufficiently large such that it had to be solved numerically. Deuflhard, Bornemann¹⁶ and Demmel¹⁷ give more detailed descriptions of these numerical methods.

Recently, Slaba *et al.*^{18,19} and Heinbockel *et al.*²⁰ developed three methods for solving the FB model which they called the collocation method, the fixed-point series method, and Wilson's method. The latter two methods are both based on Neumann series solutions wherein each term of the series solves a simple set of equations related to the original model. The work allowed for intensive verification of the multigroup method, and the collocation method was identified as the most accurate and computationally efficient.¹⁹ Slaba¹⁹ also indicated that a combination of the methods could be used to obtain a computationally efficient Neumann series solution to the DC model.

Finally, despite all of the attention given to neutron transport models and methods, accurately coupling these models back into HZETRN remained unresolved. The impact of such a coupling has not been previously studied in detail and must be examined if any of the neutron transport models are to be used in design studies.

In this paper, we first give a summary of the neutron transport models and methods developed thus far and present an efficient method for solving the DC model. Comparisons are made between the FB and DC models and the Monte Carlo codes HETC-HEDS^{21,22} and FLUKA.^{23,24} The impact of decoupling low energy neutrons from the light ion transport procedure in HZETRN is also examined, and a first order correction is presented. Fluence spectra and dose quantities are given to exhibit the accuracy of the proposed correction.

HZETRN

The one-dimensional Boltzmann transport equation for charged and neutral particles with the continuous slowing down and straight-ahead approximations is given as²

$$B[\phi_j] = \sum_k \int_E^\infty \sigma_{jk}(E, E') \phi_k(x, E') dE', \quad (1)$$

with the linear differential operator

$$B[\phi_j] \equiv \left[\frac{\partial}{\partial x} - \frac{1}{A_j} \frac{\partial}{\partial E} S_j(E) + \sigma_j(E) \right] \phi_j, \quad (2)$$

where ϕ_j is the fluence of type j ions at depth x with kinetic energy E , A_j is the atomic mass of a type j particle, $S_j(E)$ is the stopping power of a type j ion with energy E , $\sigma_j(E)$ is the total macroscopic cross section for a type j particle with energy E , and $\sigma_{jk}(E, E')$ is the

macroscopic production cross section for interactions in which a type k particle with energy E' produce a type j particle with energy E . Macroscopic cross sections are obtained by multiplying the corresponding microscopic cross section by the target particle mass density.^{2,19} Hereafter, it is assumed that all cross sections are macroscopic whether it is explicitly written or not.

Wilson *et al.*,²⁻⁶ obtained approximate solutions to equation (1) by introducing the scaled quantities

$$\psi_j(x, r) = \nu_j S_p(E) \phi_j(x, E) \quad (3)$$

$$s_{jk}(r, r') = S_p(E) \sigma_{jk}(E, E'), \quad (4)$$

where $S_p(E)$ is the proton stopping power, r is the residual proton range

$$r = \int_0^E \frac{dE'}{S_p(E')}, \quad (5)$$

and the scaling parameter $\nu_j = Z_j^2 / A_j$. For neutrons, ν is taken as unity in fluence scaling relations and zero in range scaling relations. This will be explained in more detail shortly. Equation (1) is now given in terms of the variables x and r as

$$\begin{aligned} & \left[\frac{\partial}{\partial x} - \nu_j \frac{\partial}{\partial r} S_p(E) + \sigma_j(r) \right] \psi_j(x, r) \\ & = \sum_k \frac{\nu_j}{\nu_k} \int_r^\infty s_{jk}(r, r') \psi_k(x, r') dr', \end{aligned} \quad (6)$$

which can be inverted using the method of characteristics²⁵ and written as the Volterra type integral equation³

$$\begin{aligned} \psi_j(x, r) &= e^{-\zeta_j(r, x)} \psi_j(0, r + \nu_j x) \\ &+ \sum_k \frac{\nu_j}{\nu_k} \int_0^x \int_{r+\nu_j x'}^\infty e^{-\zeta_j(r, x')} s_{jk}(r + \nu_j x', r') \\ &\times \psi_k(x - x', r') dr' dx', \end{aligned} \quad (7)$$

with

$$\zeta_j(r, x) = \int_0^x \sigma_j(r + \nu_j t) dt. \quad (8)$$

Note that ν_j in equation (3) and ν_j / ν_k in equation (6) are both fluence scaling relations, and $\nu_n = 1$ in both cases. Conversely, wherever ν appears as the argument of a fluence or cross section in equations (7) and (8) it is a range scaling relation and $\nu_n = 0$.

From here, the problem is split into two parts: heavy ions ($A > 4$) and light ions ($A \leq 4$). For heavy ions, it is noted that projectile fragments have energy and direction very near that of the projectile, while target fragments are

produced nearly isotropically with low energy and travel only a short distance before being absorbed. This approximate decoupling of target and projectile fragments is discussed in detail by Wilson *et al.*² and suggests that target fragments can be neglected in the heavy ion transport procedure (they are accounted for in dose calculations however). The production cross section can now be recast as

$$s_{jk}(r, r') = \sigma_{jk}(r) \delta(r - r'). \quad (9)$$

Equation (9) physically describes the nearly equal energy (or velocity) of the projectile and secondary particles. The final marching procedure for heavy ions was developed by Wilson *et al.*³ as

$$\begin{aligned} \psi_j(x+h, r) = & e^{-\zeta_j(r, h)} \psi_j(x, r + v_j h) \\ & + \sum_{k>j} \frac{v_j}{v_k} \sigma_{jk} \left(r + v_j \frac{h}{2} \right) \\ & \times \psi_k \left(x, r + (v_j + v_k) \frac{h}{2} \right) \\ & \times \left[\frac{e^{-\sigma_j \left(r + v_j \frac{h}{2} \right) h} - e^{-\sigma_k \left(r + (v_j + v_k) \frac{h}{2} \right) h}}{\sigma_k \left(r + (v_j + v_k) \frac{h}{2} \right) - \sigma_j \left(r + v_j \frac{h}{2} \right)} \right] \\ & + O(h^2). \end{aligned} \quad (10)$$

For light ions, both projectile and target fragments are included in the transport procedure. The broad energy distribution in collision events also indicates that equation (9) cannot be used. The final marching procedure for light ions was also developed by Wilson *et al.*²⁻⁶ as

$$\begin{aligned} \psi_j(x+h, r) = & e^{-\zeta_j(r, h)} \psi_j(x, r + v_j h) \\ & + \sum_k \frac{v_j}{v_k} \int_{r+v_j h/2}^{\infty} e^{-\zeta_j \left(r, \frac{h}{2} \right) - \zeta_k \left(r', \frac{h}{2} \right)} \\ & \times F_{jk}^{\Delta}(r, r'; h) \psi_k \left(x, r' + v_k \frac{h}{2} \right) dr' \\ & + O(h^2), \end{aligned} \quad (11)$$

where the integrand has been simplified using

$$F_{jk}^{\Delta}(r, r'; h) = \int_0^h s_{jk}(r + v_j z, r') dz. \quad (12)$$

The nature of the boundary condition, or environment, determines how equations (10) and (11) are evaluated and coupled. For most SPE environments, there are a negligible number of heavy ion projectiles, and only equation (11) is evaluated. For GCR environments, equation (10) is evaluated for heavy ions. Equation (11) is evaluated for light ions, and the summation term appearing in equation (10) is added. The summation is taken only over heavy ion projectiles, and it physically accounts for light ion production from heavy ion projectiles.

The marching equations (10) and (11) will be referred to throughout this paper as the HZETRN marching algorithm, with the proper equations evaluated and coupled for a given environment. It is important to note also that all particles, including neutrons, are propagated in the straight-ahead direction in the HZETRN marching algorithm.

NEUTRON TRANSPORT MODELS

To derive the neutron transport models, we first decompose the particle fluence and neutron production cross section into straight-ahead and isotropic components. This approximation is justified by Wilson *et al.*² who showed that projectile fragments are produced with energy and direction very near that of the projectile, while target fragments are produced nearly isotropically with very low energy. For particle fluences, the decomposition is given simply as⁷

$$\phi_j(x, E) = \phi_j^{iso}(x, E) + \phi_j^{SA}(x, E). \quad (13)$$

To decompose the neutron production cross section, we first distinguish between the nuclear reactive and elastic parts

$$\sigma_{nk}(E, E') = \sigma_{nk}^r(E, E') + \sigma_{nk}^{el}(E, E'), \quad (14)$$

where $\sigma_{nk}^{el}(E, E') = 0$ for $k \neq n$. The angularly dependent nuclear reactive neutron production cross section can be represented as⁷

$$\hat{\sigma}_{nk}^r(E, E', \Omega, \Omega') = g(A_T, E, \theta) \sigma_{nk}^r(E, E'), \quad (15)$$

with²⁶

$$g(A_T, E, \theta) = \begin{cases} Ne^{-\theta^2/\lambda} & , 0 \leq \theta \leq \pi/2 \\ Ne^{-\pi^2/4\lambda} & , \pi/2 < \theta \leq \pi \end{cases} \quad (16)$$

and $\lambda = (120 + 0.36A_T)/E$, where E is the produced neutron energy in MeV, A_T is the atomic mass of the target nucleus, θ is the production angle with respect to the direction of propagation, and N is a normalization constant such that

$$2\pi \int_0^\pi g(A_T, E, \theta) d\theta = 1. \quad (17)$$

The parameterization constants, 120 and 0.36 have units MeV and MeV/amu respectively so that λ is dimensionless.

The nuclear reactive neutron production cross section can now be decomposed into forward (scattering angle $\theta \in [0, \pi/2]$) and backward (scattering angle $\theta \in (\pi/2, \pi]$) components

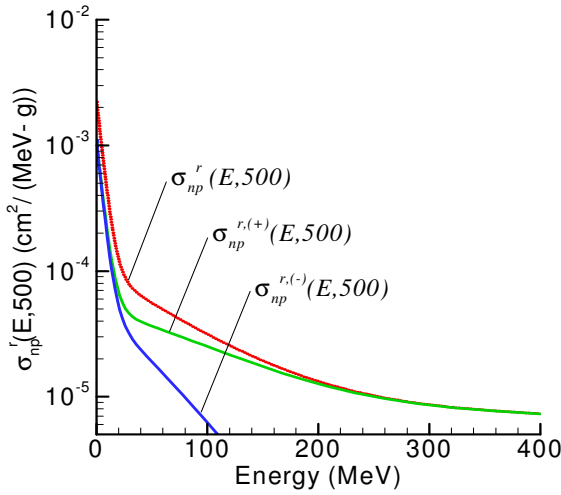


Fig. 1 Forward, backward, and total neutron nuclear reactive production cross section for a 500 MeV proton projectile and an Aluminum target.

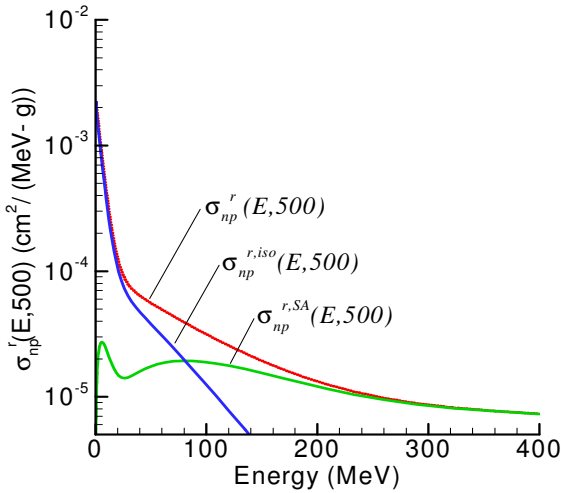


Fig. 2 Straight ahead, isotropic, and total neutron nuclear reactive production cross section for a 500 MeV proton projectile and an Aluminum target.

$$\begin{aligned}\sigma_{nk}^r(E, E') &= F^{(+)}(A_T, E)\sigma_{nk}^r(E, E') \\ &+ F^{(-)}(A_T, E)\sigma_{nk}^r(E, E') \\ &\equiv \sigma_{nk}^{r,(+)}(E, E') + \sigma_{nk}^{r,(-)}(E, E'),\end{aligned}\quad (18)$$

where the forward and backward coefficients are

$$F^{(+)}(A_T, E) = \int_0^{\pi/2} g(A_T, E, \theta) d\theta \quad (19)$$

$$F^{(-)}(A_T, E) = 1 - F^{(+)}(A_T, E). \quad (20)$$

The straight-ahead¹² and isotropic coefficients are therefore defined as¹²

$$F^{SA}(A_T, E) = 1 - F^{iso}(A_T, E) \quad (21)$$

$$F^{iso}(A_T, E) = 2F^{(-)}(A_T, E), \quad (22)$$

so that the nuclear reactive neutron production cross section can be expressed in terms of isotropic and straight-ahead components

$$\begin{aligned}\sigma_{nk}^r(E, E') &= F^{SA}(A_T, E)\sigma_{nk}^r(E, E') \\ &+ F^{iso}(A_T, E)\sigma_{nk}^r(E, E') \\ &\equiv \sigma_{nk}^{r,SA}(E, E') + \sigma_{nk}^{r,iso}(E, E').\end{aligned}\quad (23)$$

The decompositions in equations (18) and (23) are depicted in Figs. 1 and 2 for a 500 MeV proton projectile and an Aluminum target. It should be noted in Fig. 2 that the straight-ahead component of the nuclear reactive neutron production cross section is dominant at high fragment energies, while the isotropic component is dominant at low fragment energies as suggested earlier.

Equations (13), (14) and (23) are substituted into equation (1) and the HZETRN marching algorithm is used to solve

$$B[\phi_j^{SA}] = \sum_k \int_E^\infty \kappa_{jk}^{SA}(E, E') \phi_k^{SA}(x, E') dE', \quad (24)$$

where the production cross section $\kappa_{jk}(E, E')$ is piecewise defined as

$$\kappa_{jk}^{SA}(E, E') = \begin{cases} \sigma_{nk}^{r,SA}(E, E') + \sigma_{nk}^{el}(E, E') & , j = n \\ \sigma_{jk}(E, E') & , j \neq n \end{cases} \quad (25)$$

The only difference between equations (1) and (24) is the form of the neutron production section; equation (1) uses the total nuclear reactive neutron production cross section, while equation (24) uses only the straight-ahead component. Fig. 2 suggests that neutron fluences obtained from equation (24) will have attenuated low energy spectra, and examination of the HZETRN marching algorithm indicates a residual attenuation will occur in the low energy light ion spectra as well. This behavior is evident in Fig. 3. More will be said about this later in the paper as well.

We are now left to solve

$$\begin{aligned}B[\phi_n^{iso}] &= \sum_{k \neq n} \int_E^\infty \sigma_{nk}(E, E') \phi_k^{iso}(x, E') dE' \\ &+ \int_E^\infty \sigma_{nn}(E, E') \phi_n^{iso}(x, E') dE' \\ &+ \eta_n(x, E),\end{aligned}\quad (26)$$

with the isotropic neutron source term

$$\eta_n(x, E) = \sum_k \int_E^\infty \sigma_{nk}^{r,iso}(E, E') \phi_k^{SA}(x, E') dE'. \quad (27)$$

The isotropic component of the charged particles is obtained by solving