CONF-880601--41

DE88 012920

Deterministic Transport Calculations of Dose Profiles Due to Proton Beam Irradiation,

W. L. Filippone (Univ of Arizona), M. S. Smith, R. T. Santoro, T. A. Gabriel, R. G. Alsmiller, Jr. (ORNL)

Charged-particle transport calculations are most often carried out using the Monte Carlo technique. For example, the TIGER (Ref. 1) and EGS (Ref. 2) codes are used for electron transport calculations, while HETC (Ref. 3) models the transport of protons and heavy ions.

In recent years there has been considerable progress in deterministic models of electron transport.[4-9] Many of these models are also applicable to protons. In this paper we present discrete ordinates solutions to the Spencer-Lewis[10-12] equation for protons. In its present form, our code calculates the energy deposition profile and primary proton flux in x-y geometry due to proton beam irradiation. Proton energies up to 0.4 GeV are permissible.

The Spencer-Lewis equation for the proton angular flux $\phi(x,y,s,\hat{\Omega})$ is

$$\left[\frac{\partial}{\partial s} + \Omega_x \frac{\partial}{\partial x} + \Omega_y \frac{\partial}{\partial y} + \sigma(s)\right]\phi(x,y,s,\hat{\Omega}) = \int_{4\pi} \sigma(s,\hat{\Omega}' \rightarrow \hat{\Omega})\phi(x,y,s,\hat{\Omega}')\,d\Omega' + Q(x,y,s,\hat{\Omega}) \ , \quad (1)$$

where

Ω_x, Ω_y = x and y components of the velocity direction, respectively

$\sigma(s)$ = total interaction cross section, including nuclear and coulomb collisions

$\sigma(s,\hat{\Omega}' \rightarrow \hat{\Omega})$ = differential scattering cross section for nuclear and coulomb collisions

s = path length, which is used as our energy variable in the continuous slowing down approximation (CSDA).

Once ϕ of $(x,y,s,\hat{\Omega})$ is found, the energy deposition profile (EDP) can be given by

$$\mathrm{EDP}(x,y) = \int \left|\frac{dE}{ds}\right| \Phi(x,y,s)\,ds \ , \quad (2)$$

where $|dE/ds|$ is the proton stopping power, and

$$\Phi(x,y,s) = \int_{4\pi} \phi(x,y,s,\hat{\Omega})\,d\hat{\Omega} \quad (3)$$

is the scalar flux.

For energies below 0.4 GeV, protons lose energy primarily through coulomb collisions with electrons. This is modeled using the CSDA. The required stopping powers are obtained from the computer code SPAR (Ref. 13), which has been included in the main program as a subroutine.

CONF-880601--41

DETERMINISTIC TRANSPORT CALCULATIONS OF DOSE PROFILES DUE TO PROTON BEAM IRRADIATION*

W. L. Filippone
Department of Nuclear Engineering
University of Arizona
Tucson, Arizona 85721

M. S. Smith, R. T. Santoro,
T. A. Gabriel, and R. G. Alsmiller, Jr.
Oak Ridge National Laboratory†
Oak Ridge, Tennessee 37831

Presentation given at the ANS Annual Meeting in San Diego (1988).

* This work was partially sponsored by the U.S. Department of Defense, Air Force Weapons Laboratory, and the University of Arizona

† Operated by Martin Marietta Energy Systems, Inc., under contract DE-AC05-84OR21400, U.S. Department of Energy

Nuclear coulomb collisions do not produce significant energy losses; however, they can cause (normally very small) angular deflections. These collisions are modeled using Rutherford scattering with the screening parameter given by Moliere.[14] As with electron transport calculations, the scattering integral in Eq. (1) is carried out numerically using discrete directions. Due to the extreme anisotropy (even more so than for electrons) of proton coulomb scattering, however, good accuracy would require a huge number of discrete directions rendering numerical solutions unfeasible on present-day computers. To overcome this problem, the SMART scattering matrix technique[9] developed for electron transport is used. This scattering matrix enables us to model a very large number of minute deflections by relatively few larger deflections.

At the present time, our code treats only primary protons. Primary protons are removed through (p,n) and (p,p) nuclear collisions. The cross sections for these reactions are obtained from the NCDATA code[15] that interpolates values from analytic fits to the nonelastic cross-section data generated by Bertini[16,17] using an internuclear-cascade model.

Because of the statistical nature of charged-particle interactions, all protons of a given energy will not have identical ranges. This phenomenon is referred to as range straggling. Coulomb collisions with nuclei contribute to straggling by imposing a variety of angular deflections to the proton trajectories. A somewhat larger contribution comes from fluctuations in the rate of energy loss due to electron collisions. The former cause of straggling is modeled through our treatment of multiple scattering from nuclei; however, the CSDA implies the same stopping power for all protons of a given energy so that the latter type of straggling is not modeled by the Spencer-Lewis equation. In most cases, straggling can be neglected; however, it can be significant for problems involving monoenergetic sources. For these problems an analytic first collision source[18] (made feasible by the relatively large effective mean-free-path obtained from SMART scattering theory[18]) is used. To simulate straggling from energy loss fluctuations, source particles of the same energy are given slightly different stopping powers. Typically, ten different values are used. These values are chosen such that the average stopping power and the percentage of range straggling (available from Ref. 19) are preserved.

Dose profiles have been calculated for several source and target geometries. Figure 1 shows S_N and Monte Carlo results for the dose profile integrated over the y direction in a two-dimensional target due to a normally incident beam of 200-MeV protons. The target consists of an aluminum region ($1.5\text{ cm} < x < 5\text{ cm}$, $0 < y < 1.87\text{ cm}$) sandwiched between two lead regions ($0 < x < 1.5\text{ cm}$, $5.0\text{ cm} < x < 7.0\text{ cm}$, $0 < y < 1.87\text{ cm}$) with the source located at (0.936 cm).

The S_N and Monte Carlo results are in excellent agreement, except near the peak. The discrepancy there is probably due to the fact that the HETC calculations do not include multiple nuclear scattering, to diamond-differencing errors, and to differences in the treatment of straggling.

The results for Fig. 1 do not include attenuation from inelastic nuclear collisions. When these collisions are included there is an ~25% reduction in the peak height, which is consistent with the probabilities of nuclear collision given in Ref. 19.

The next phase of code development will be to include secondary protons. Since the CSDA does not apply to inelastic nuclear collisions, it will be assumed that each inelastic collision kills the primary proton and produces a new proton that shows up in $Q(x,y,s,\hat{\Omega})$ at the appropriate s value. The necessary differential cross sections (p,p), (p,n), and (n,p) will be interpolated using NCDATA.

Since protons tend to travel in straight lines, it may appear that ray effects could be significant. No ray effects have been observed thus far, however, and nuclear collision, first collision sources, and the effects coupled neutron-proton transport should help prevent this problem.

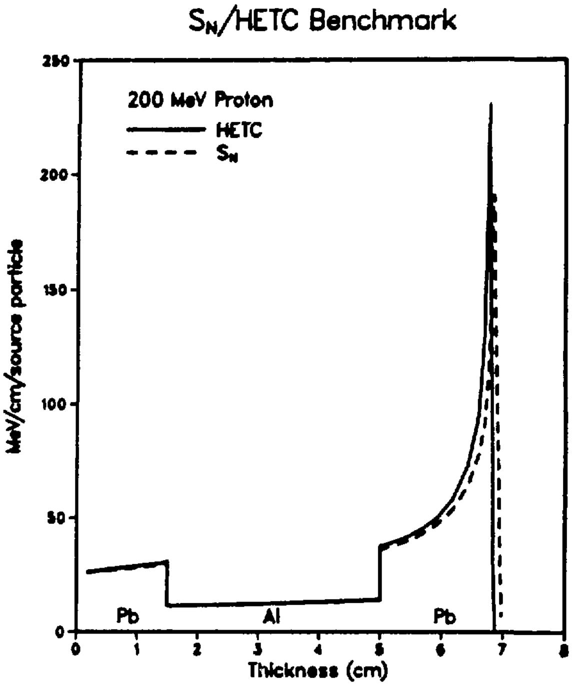

Fig. 1. Energy deposition profile calculated using the Monte Carlo (HETC) and S_N methods.

1. J. A. HALBLEIB, T. A. MEHLORN, "ITS: The Integrated TIGER Series of Coupled Electron/Photon Monte Carlo Transport Codes," SAND84-0573, Sandia National Labs. (Nov. 1984).

2. W. R. NELSON, A. HIRAYAMA, D. W. O. ROGERS, "The EGS4 Code System," SLAC-265, Stanford Linear Accelerator Center, Stanford, California (Dec. 1985).

3. K. C. CHANDLER, T. W. ARMSTRONG, "Operating Instructions for the High Energy Transport Code HETC," ORNL-4744, Oak Ridge National Lab. (1972).

4. D. E. BARTINE, R. G. ALSMILLER, Jr., F. R. MYNATT, W. W. ENGLE, Jr., J. BARISH, *Nucl. Sci. Eng.*, **48**, 159 (1972).

5. J. E. MOREL, *Nucl. Sci. Eng.*, **79**, 340 (1981).

6. J. E. MOREL, *Nucl. Sci. Eng.*, **91**, 324 (1985).

7. W. L. FILIPPONE, M. S. SMITH, S. WOOLF, J. C. GARTH, *Nucl. Sci. Eng.*, **95**, 22 (1987).

8. W. L. FILIPPONE, S. WOOLF, J. C. GARTH, *IEEE Trans. Nucl. Sci.*, **NS-34**, 1564 (1987).

9. W. L. FILIPPONE, "The Theory and Application of SMART Electron Scattering Matrices," to appear in *Nucl. Sci. Eng.*

10. H. W. LEWIS, *Phys. Rev.*, **78**, 526 (1950).

11. L. V. SPENCER, *Phys. Rev.*, **98**, 1597 (1955).

12. W. L. FILIPPONE, *TTSF*, **15**, 5, 624 (1986).

13. T. W. ARMSTRONG, K. C. CHANDLER, "SPAR, A FORTRAN Program for Computing Stopping Powers

and Ranges for Muons, Charged Pions, Protons, and Heavy Ions," ORNL-4869, UC 32-Mathematics and Computers, Oak Ridge National Lab. (1973).

14. G. MOLIERE, *Z. Naturforsch*, **2A**, 133 (1947).

15. R. G. ALSMILLER, Jr., J. BARRISH, "NCDATA—Nuclear Collision Data for Nucleon-Nucleus Collisions in the Energy Range 25 to 400 MeV," ORNL-4220, UC-34-Physics, Oak Ridge National Lab. (1968).

16. H. W. BERTINI, *Phys. Rev.*, **131**, 1801 (1963); with erratum *Phys. Rev.*, **138**, AB2 (1965).

17. H. W. BERTINI, *Nucl. Phys.*, **87**, 138 (1966).

18. W. E. FILIPPONE, S. WOOLF, J. C. GARTH, *Trans. Am. Nucl. Soc.*, **55**, 356 (1987).

19. J. F. JANNI, "Calculations of Energy Loss, Range, Path Length, Straggling, Multiple Scattering, and the Probability of Inelastic Nuclear Collisions for 0.1- to 1000-MeV Protons," AFWL-TR-65-150, Air Force Weapons Lab., Kirtland AFB, New Mexico (1966).

5. Transport of Cosmic Ray Nuclei in Various Materials, *R. Silberberg, C. H. Tsao (E. O. Hulburt Center), John R. Letaw (Severn Communications)*, *invited*

INTRODUCTION

Studies of cosmic-ray transport in materials have traditionally provided astrophysicists with detailed tests of processes related to the origin of the chemical elements. Cosmic rays are a sample of material recently injected into the galaxy. They are accelerated to high energies (generally between 10 MeV and 10 GeV per nucleon) by mechanisms associated with supernova explosions. Consisting of all stable and long-lived nuclei, they provide direct insight into ongoing nucleosynthesis and mass-ejection processes.

The passage of cosmic rays through meteorites, lunar soil, the interstellar medium, and the Earth's atmosphere causes nuclear spallation reactions. These reactions produce numerous isotopes that are of interest in a variety of scientific disciplines. For example, cosmic-ray interactions with the interstellar gas are responsible for much of the lithium, beryllium, and boron in the universe. The extent of this production process places important constraints on big-bang nucleosynthesis models. Cosmic-ray interactions with the Earth's atmosphere are the continuous source of ^{14}C and ^{10}Be, which is measured in radioactive dating studies.

More recently, cosmic-ray heavy ions have become a concern in space radiation effects analyses. Heavy ions rapidly deposit energy and create dense ionization trails as they traverse materials. Collection of the free charge disrupts the operation of microelectronic circuits. This effect, called the single-event upset, can cause a loss of digital data. Passage of high linear energy transfer particles through the eyes has been observed by Apollo astronauts. These heavy ions have great radiobiological effectiveness and are the primary risk factor for leukemia induction on a manned Mars mission.[1]

Models of the transport of heavy cosmic-ray nuclei through materials depend heavily on our understanding of the cosmic-ray environment, nuclear spallation cross sections, and computer transport codes. Our group has initiated and pursued the development of a full capability for modeling these transport processes.[2-4] A recent review of this ongoing effort is presented in Ref. 5. In this paper, we discuss transport methods and present new results comparing the attenuation of cosmic rays in various materials.

DESCRIPTION OF WORK

Transport of heavy cosmic-ray nuclei through shielding materials is computed in the straight-ahead approximation. In this approximation, the velocity of nuclei and their fragments are constant through a nuclear reaction. The straight-ahead approximation fails for low-energy, light nuclei, but is excellent for cosmic-ray transport modeling because (a) cosmic rays have mean energy per nucleon exceeding 1 GeV, (b) heavy nuclei are the principal cause of significant radiation effects, and (c) protons interact rarely in materials. Effects dominated by proton interactions are best simulated by a full-scale Monte Carlo calculation.

Our transport code obtains the exact, numerical solution of the following equation:

$$\frac{\partial J_i}{\partial x} = -J_i\left(\frac{N}{\rho}\right)\sigma_i + \sum_{j>i} J_j\left(\frac{N}{\rho}\right)\sigma_{ij} + \frac{\partial}{\partial E}\left[J_i\left(\frac{dE}{dx}\right)_i\right] . \quad (1)$$

This equation describes the change in the flux as it traverses a path length x ($g \cdot cm^{-2}$) in a given material. The value $J_i(E)$ is the differential flux of nuclei of type i at energy E. It has been found sufficient to treat only the first 28 elements (through nickel) in the energy range from 1 MeV to 100 GeV per nucleon for many problems. Transport of individual isotopes is unnecessary for space radiation effect applications; however, we treat individual isotopes in modeling observed isotopic abundances in cosmic-ray detectors and accelerator applications.

On the right side, the first term represents the loss of nuclei of type i due to spallation. The value σ_i is the total inelastic cross section of nuclide i in the target material, and N and ρ are the number and mass densities, respectively, of the target material. The second term represents the production of nuclide i from spallation of heavier nuclides j. The quantity σ_{ij} is the partial cross section of nuclide j into i. The third term represents the ionization losses that continuously shift flux to lower energies.

The cross sections σ_i and σ_{ij} are calculated using semi-empirical methods developed by Silberberg, Tsao, and Letaw and reported in Refs. 4, 6, 7, and 8. We are now completing the formulation of the nucleus-nucleus cross section given by

$$\sigma(N_1,N_2) = \sigma(N_1,p) \times S_c \times \epsilon_L \times \epsilon_\Delta \times \epsilon_1 , \quad (2)$$

where $\sigma(N_1,N_2)$ is the partial cross section for fragmenting nuclide N_1 in collisions with target N_2, $\sigma(N_1,p)$ is that for N_1 colliding with protons, S_c is a scaling factor, ϵ_1 is the enhancement factor for single-nucleon stripping, ϵ_L is the enhancement factor for the production of light nuclei 3 ≤

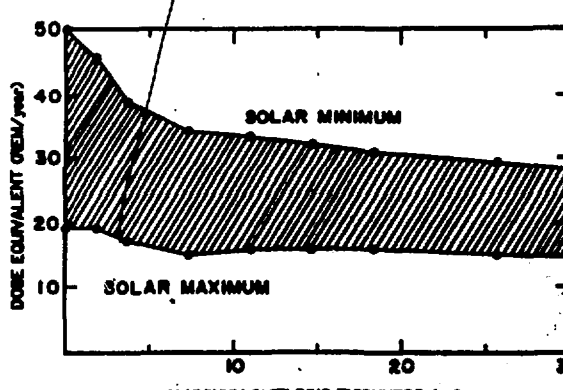

Fig. 1. Galactic cosmic radiation dose to red bone marrow compared with aluminum shielding thickness.