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ADVANCES IN SPACE RESEARCH (a COSPAR publication)

Advances in Space Research 45 (2010) 884–891

www.elsevier.com/locate/asr

Proton lateral broadening distribution comparisons between GRNTRN, MCNPX, and laboratory beam measurements

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Received 14 May 2009; received in revised form 6 August 2009; accepted 13 August 2009

Abstract

Recent developments in NASA's deterministic High charge (Z) and Energy TRaNsport (HZETRN) code have included lateral broadening of primary ion beams due to small-angle multiple Coulomb scattering, and coupling of the ion-nuclear scattering interactions with energy loss and straggling. This new version of HZETRN is based on Green function methods, called GRNTRN, and is suitable for modeling transport with both space environment and laboratory boundary conditions. Multiple scattering processes are a necessary extension to GRNTRN in order to accurately model ion beam experiments, to simulate the physical and biological-effective radiation dose, and to develop new methods and strategies for light-ion radiation therapy. In this paper we compare GRNTRN simulations of proton lateral broadening distributions with beam measurements taken at Loma Linda University Proton Therapy Facility. The simulated and measured lateral broadening distributions are compared for a 250 MeV proton beam on aluminum, polyethylene, polystyrene, bone substitute, iron, and lead target materials. The GRNTRN results are also compared to simulations from the Monte Carlo MCNPX code for the same projectile-target combinations described above.

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Keywords: Radiation transport; Ion beam measurements; Multiple scattering; Radiobiology; GRNTRN

1. Introduction

GReeN function TRaNsport (GRNTRN) is a new version of NASA's deterministic High charge (Z) and Energy TRaNsport (HZETRN) code that is based on non-perturbative Green function techniques for the transport of charged particles through target media [\(Tweed et al.,](#page--1-0) [2004, 2005](#page--1-0)). The computational transport procedures in HZETRN were developed for space environment boundary conditions consisting of omni-directional particle flux with continuous energy spectra ([Wilson et al., 1991\)](#page--1-0). Ground-based laboratory beam experiments, on the other hand, are described by the transport of directed-beams of ions with quasi-monochromic energy. The advantage of the Green function approach, and the motivation for GRNTRN development, is the ease and flexibility by which both ground-based laboratory and space environment boundary conditions can be incorporated into a single theoretical formulation. Moreover, the Green function method enables detailed simulations of the response of particle spectrometer devices, which are used to analyze laboratory beam experiments ([Walker et al., 2005\)](#page--1-0).

Because ion beams in laboratory experiments are quasi mono-directional, incorporating off-axis dispersion of the primary ion beam is an important feature that needs to be included in ion beam transport codes. The beam broadening mechanism included in GRNTRN is attributed to small-angle multiple Coulomb scattering of the incident ion beam by the target media nuclei [\(Mertens et al.,](#page--1-0)

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^{0273-1177/\$36.00} Published by Elsevier Ltd. on behalf of COSPAR. doi:[10.1016/j.asr.2009.08.013](http://dx.doi.org/10.1016/j.asr.2009.08.013)

[2007](#page--1-0)). While the effects of multiple scattering are negligible in the omni-directional space radiation environment, multiple scattering effects must be included in directed-beam applications and ground-based laboratory transport code simulations.

[Mertens et al. \(2007\)](#page--1-0) presented the theoretical formulation and computation procedures for incorporating smallangle multiple Coulomb scattering into the GRNTRN code. The GRNTRN multiple scattering interactions and transport include a self-consistent coupling of ion-nucleus scattering with ionization energy loss and straggling. Initial benchmark studies included comparisons of beam broadening characteristics with Monte Carlo simulations and laboratory experiments reported by [Noshad and Givechi](#page--1-0) [\(2005\)](#page--1-0) for a 60 MeV proton beam on muscle tissue.

In this paper we expand upon our initial benchmark studies and compare proton lateral broadening distributions with beam experiments conducted by [Moyers \(2005\)](#page--1-0) at the Loma Linda University Proton Treatment Facility (LLUPTF). In the LLUPTF experiments, a 250 MeV proton beam was incident upon phantom targets representative of low- (≤ 1 g/cm³), medium- (1–5 g/cm³), and high-density $($ >5 g/cm³ $)$ materials. The low-density materials are air, high-density polyethylene (HDPE), and clear cross-linked polystyrene (CLPS). The medium-density materials are RMI bone and aluminum (Al). For reference, the RMI bone composition, in percent by weight, consists of 3.15% hydrogen, 31.58% carbon, 1% nitrogen, 37.41% oxygen, 0.05% chlorine, and 26.81% calcium. The high-density materials are iron (Fe) and lead (Pb). We compare GRNTRN/ LLUPTF lateral broadening distributions for all proton-target materials listed above. Moreover, we compare the Monte Carlo MCNPX code simulations of the lateral beam broadened full-width at half-max (FWHM) reported by [Moyers](#page--1-0) [\(2005\)](#page--1-0) with corresponding GRNTRN simulations for the same proton-target combinations described above.

2. GRNTRN multiple scattering formulation

In this section, we outline the main features of the transport methodology implemented in GRNTRN for computing the lateral broadening distribution of the primary ion beam due to small-angle multiple Coulomb ion-nuclear scattering. The details of the theoretical formulation and computational procedures were presented in an earlier report ([Mertens et al., 2007](#page--1-0)).

At LLUPT, the lateral broadening distributions were measured with an extended dose range radiographic film. To compare with these measurements, we computed the off-axis dose distributions by factoring it into an on-axis dose distribution modulated by an off-axis beam broadening function [\(Hogstrom et al., 1981\)](#page--1-0), such that

$$
d(x, y, z) = f(x, y, z)d(z),\tag{1}
$$

where $d(z)$ is the on-axis dose distribution and $f(x, y, z)$ is the off-axis beam broadening function. The on-axis dose distribution is given by the expression

$$
d(z) = K \int_0^\infty S(E)\Phi(z, E)dE,
$$
\n(2)

where $S(E)$ is the stopping power, $\Phi(z, E)$ is the on-axis spectral flux distribution computed from a second-order energy moment expansion of the Boltzmann transport equation ([Wilson and Tai, 2000; Wilson et al., 2002](#page--1-0)), and K is a unit conversion factor. Assuming cylindrical symmetry, the off-axis broadening function is given by

$$
f(x, y, z) = \frac{1}{\pi \langle r^2(z) \rangle} \exp\left(-\frac{(x^2 + y^2)}{\langle r^2(z) \rangle}\right).
$$
 (3)

Moreover, the transport integral for the radial broadening statistical moment is

$$
\langle r^2(z)\rangle = \langle r^2(0)\rangle + \int_0^z (z-z')^2 \frac{d\langle \theta^2(z')\rangle}{dz'} dz'.
$$
 (4)

In the above equation, $\langle r^2(0) \rangle$ is the initial radial broadening of the incident ion beam, which assumes there are no initial angular broadening and radial-angular correlation in the incident ion beam – i.e., all incident ions are propagating parallel to one another. The scattering power in (4) is given by

$$
\frac{d\langle\theta^2(z)\rangle}{dz} = 4\pi Z_P^2 \frac{(r_e\mu_e)^2}{(v(z)p(z))^2} \sum_m \rho_A(m) Z_T(m) (Z_T(m) + 1) \times \ln[\theta_r^2(m) + 1] - 1 + [\theta_r^2(m) + 1]^{-1},
$$
\n(5)

where

$$
\theta_r \equiv \frac{\theta_u}{\theta_l} = \left[181 Z_T^{-1/3} \left(\frac{Z_T}{A_T} \right)^{1/6} \right]^2. \tag{6}
$$

In Eqs. (5) and (6), the variables are defined as follows: A_T is the target atomic mass number, Z_T and Z_P are the target and projectile atomic charge numbers, respectively, r_e is the classical electron radius, μ_e is the electron rest mass, v and p are the projectile velocity and momentum, respectively, ρ_A is the number of atoms per gram, θ_u and θ_l are the upper and lower limits of the scattering angle consistent with small-angle Coulomb scattering, and the summation is over m, the elemental constituents of the target material.

Ionization energy loss is implicitly coupled to the multiple scattering transport through the depth dependence of the projectile velocity and momentum in (5). Assuming the continuous slowing down approximation, the mean energy of the ion beam after propagating a longitudinal distance z into the target material is given by the usual range-energy relations [\(Wilson et al., 1991\)](#page--1-0). The velocity and momentum of the projectile at each propagation depth $-z$ in (5) can be evaluated using the mean energy and the relativistic kinematic relations.

In order to achieve a self-consistent coupling between multiple scattering transport and energy loss, the influence of multiple scattering on the mean energy must also be included, in addition to the influence of energy loss on multiple scattering implicit in (5).

The mean energy of the projectile beam at physical depth – z is related to the residual range via the usual range-energy relation

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