Physica Medica 31 (2015) 912–921

Contents lists available at ScienceDirect

Physica Medica

journal homepage: http://www.physicamedica.com

Original Paper

# Deterministic model for the transport of energetic particles: Application in the electron radiotherapy

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ARTICLE INFO

*Article history:*
Received 19 December 2014
Received in revised form 3 July 2015
Accepted 13 July 2015
Available online

*Keywords:*
Radiotherapy treatment planning system
Deterministic algorithm
Electron dosimetry
Monte Carlo algorithm

ABSTRACT

A new deterministic method for calculating the dose distribution in the electron radiotherapy field is presented. The aim of this work was to validate our model by comparing it with the Monte Carlo simulation toolkit, GEANT4. A comparison of the longitudinal and transverse dose deposition profiles and electron distributions in homogeneous water phantoms showed a good accuracy of our model for electron transport, while reducing the calculation time by a factor of 50. Although the Bremsstrahlung effect is not yet implemented in our model, we propose here a method that solves the Boltzmann kinetic equation and provides a viable and efficient alternative to the expensive Monte Carlo modeling.



## Introduction

Radiotherapy is one of the most efficient cancer treatment, that delivers high dose on target volumes, despite the side effects from delivering dose on organs at risk. To improve the dose distribution, more accurate and complex radiation techniques such as the Intensity Modulated Radiotherapy (IMRT) and its derived version, the Volumetric Modulated Arctherapy (VMAT) are required. In parallel, the emergence of the Adaptative Planning approach in clinical practice allows to evaluate the dose delivered to the patient in real-time, and to therefore adapt the treatment plan during the course of radiotherapy. Along with hardware development and improvements in imaging diagnostics, these techniques emphasize the need for a more efficient and accurate dose calculation algorithm. Along with statistical methods such as the full and reduced (fast) Monte Carlo (MC) technique [1–3], alternative methods based on a deterministic approach are proposed [4–7]. These methods resolve the kinetic equations (Fokker–Planck or Boltzmann) on a regular mesh and have advantages such as reduced noise level and improved precision. However, even fast MC methods are slow and time consuming in clinical applications.

Here, we propose a new method for Boltzmann kinetic equation resolution, which combines the precision of the deterministic approach of the MC methods with the rapidity of fast simplistic methods such as the pencil beam type algorithm. This deterministic algorithm, M1, is based on a multi-group energy approach combined with a specific angular momentum closure [8]. For each energy group, the equations for two angular moments (one scalar and one vector) are closed with an algebraic relation deduced from the principle of the entropy minimization. This method is already implemented in the plasma physics, with good efficiency and sufficient accuracy, to describe the radiation transport [4] and the energetic electron transport [9]. For medical applications, we created a computing platform, KIDS (Kinetic Dose Simulation), dedicated to the specific physical processes that needed to be considered. In this article, we evaluate the accuracy of the M1 algorithm for calculating dose deposition with electron beams. Therefore, we compare the dose calculations with the electron transport M1 model to the full Monte Carlo code GEANT4 (GEometry ANd Tracking) reference simulations [10,11].

Previously developed for the plasma physics simulations, the M1 code is not yet configured to match the special medical requirements such as diverging beams, or the source-phantom distance. Hence the scope of this article is limited to the evaluation of the precision and the performance of the M1 algorithm and its utility in medical applications. This is achieved by comparing two codes with the same basic input data and parameters: a Gaussian energetic distribution of a parallel beam and a simple square field size.

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http://dx.doi.org/10.1016/j.ejmp.2015.07.148
1120-1797/

Thus, the modeling of a complete accelerator head is not required at this time, and comparisons with commercially released algorithms would be premature and not judicious. Longitudinal and transversal dose profiles for the homogeneous water phantom cases as well as the relative output factors are compared. We demonstrate an overall good match in the dose deposition profile with a very significant improvement in the simulation time compared to the MC code. The discrepancies in the dose deposition (typically less than a few percent) are explained by comparing the distribution functions of electrons in energy and angles thus opening way for further developments.

## Materials and methods

### *Particle interaction processed in M1 and relative contributions*

Modeling of the dose deposition in a medium with ionizing radiation requires the knowledge of interaction cross sections of the primary particles, (electrons in our case) and the secondary particles (electrons and photons) [12]. The following scattering processes, which the incident electrons undergo in matter, were incorporated in the M1 code:

- The elastic collisions of an electron with nuclei, which correspond to a deflection of the incident electron without energy loss (because the mass of the target nuclei is much greater than that of the electron);
- The inelastic collisions of the incident electron with the atomic electrons, which lead to an ionization and/or an excitation of atoms, and to a loss of energy of the incident particle. The soft and the hard collisions can be distinguished as follows:
  - Soft collisions occur with the outer atomic shell electrons, whose binding energies are only of a few eV. The deflection of the incident electrons is small and a relatively little amount of energy is lost;
  - Hard collisions correspond to a large transfer of energy and a large scattering angle. The deflected electrons are usually called secondary electrons or delta rays and constitute an additional source that was taken into account in the model.

The elastic collisions of electrons with atoms without energy loss are excluded from our model. This process is important only for electrons with energies comparable to the binding energy of atomic electrons. We therefore limited our transport model to electrons with energies above 10 keV, whose mean free path is comparable to spatial resolution to the order of 0.1 mm (acceptable in the practical radiotherapy).

The analytic formulations of electron scattering processes for electron-ion elastic- and inelastic- cross sections were originally described by Mott and Massey [13] and Møller [14], respectively. Furthermore, many other publications also present a detailed account of these relations [5,12,15,16].

The M1 model accounts for the electron energy losses in soft collisions in the Continuous Slowing Down (CSD) approximation [12]. The hard electron collision, being a source of secondary electrons, is described as a separate "ionization" term by Refs [17,18]. The elastic collisions with nuclei and atomic electrons (small deflections) are accounted for, in a diffusion approximation, as a graduate increase of the average angle of the electron propagation with respect to the main beam propagation direction. Such a blooming effect has a significant impact on the spatial and energetic electron distribution and hence on the deposited dose. These approximations are inherently linked to the notion of the electron mean free path – the average distance between two subsequent collisions. The CSD approximation implies that the size of energy deposition zone is larger than the electron mean free path.

A comparison of contributions of above cited interaction processes in the range of the energies that meets radiotherapy requirements, from a few keV to a few dozens of MeV in water, shows that the inelastic and elastic scattering processes have a much larger cross-sections compared to the Bremsstrahlung effect. For this reason, in a first approximation, the Bremsstrahlung effect is not implemented in our code. This is sufficient for the proof of principle demonstration of the M1 method. Although the Bremsstrahlung process is important for the correct dose calculation, its contribution varies from a few percent for lower clinical energy beams (6 to 12 MeV) to 5% for higher energy beams (20 MeV) [19,20]. This physical process is compatible with the M1 algorithm and it will be included in the future version of our code.

### *M1 method*

The deterministic kinetic M1 model, initially used in particle physics and Inertial Confinement Fusion, was implemented in the KIDS platform dedicated to medical applications.

The M1 model applies to the linearized Boltzmann kinetic equation that describes the propagation of relativistic electrons in matter. It accounts for small angle collisions with electrons and ions of the medium in the CSD diffusion approximation and with a source term $Q_I$ of secondary electrons [18]:

$$-\frac{1}{p^2}\frac{\partial}{\partial p}(p^2 f \rho S_M) + v\vec{\Omega}\cdot\nabla f = \frac{v\rho k_1}{2}L[f] + \rho Q_I[f], \tag{1}$$

where $f(\vec{r},\vec{p})$ is the fast electron distribution function depending on the coordinate $\vec{r}$, where $p = m_e v\gamma$ is the electron momentum, $v$ is its velocity, $m_e$ is the electron mass, $\gamma$ is the relativistic factor, $\vec{\Omega}$ is the unitary vector in the direction of electron propagation, $S_M$ is the stopping power (4), $k_1$ is the total angular isotropization rate (5) and $\rho = \rho(\vec{r})$ is the density of the considered medium.

The linear operator $L[f]$ related to the Laplace–Beltrami operator describes the angular scattering of the particles:

$$L[f] = \frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial f}{\partial\mu} + \frac{1}{1-\mu^2}\frac{\partial^2 f}{\partial\phi^2}, \tag{2}$$

where $\mu = cos\theta$, $\mu$ and $\phi$ being the polar and azimuthal angles of the vector $\vec{\Omega}$.

It is useful to introduce the notation $\Psi(\vec{r},\vec{\Omega},\varepsilon) = p^2 f(\vec{r},\vec{p})$, where $\varepsilon$ is the electron's kinetic energy $\varepsilon = m_e c^2(\gamma - 1)$ to present Eq. (1) as follows:

$$-\frac{\partial}{\partial\varepsilon}(\Psi\rho S_M) + \vec{\Omega}\cdot\nabla\Psi = \frac{k_1\rho}{2}L[\Psi] + \rho\tilde{Q}_I[\Psi]. \tag{3}$$

The electron stopping power $S_M$ is defined by the angle-averaged Møller cross-section $\sigma^e_{Møller}$:

$$S_M(\varepsilon) = \frac{Z}{Am_p}\frac{1}{m_e c^2}\int_{\varepsilon_B}^{(\varepsilon-\varepsilon_B)/2}\varepsilon'\sigma^e_{Møller}(\varepsilon,\varepsilon'\mu)d\varepsilon' d\mu, \tag{4}$$

where $A$ is the average mass of the medium, $Z$ is the atomic number, $m_p$ the mass of proton and $\varepsilon_B$ is the average binding energy of atomic electrons.

The effect of elastic electron scattering in the M1 model is described by the transport coefficient $k_1$, which includes two terms relating to scattering on ions and atomic electrons. Both terms are the integrals of the differential elastic cross sections by Mott and Møller (on ions and electrons, respectively) over the scattering angles. With $\mu = cos\theta$ the cosine of the scattering angle $\theta$, $k_1$ is given by: