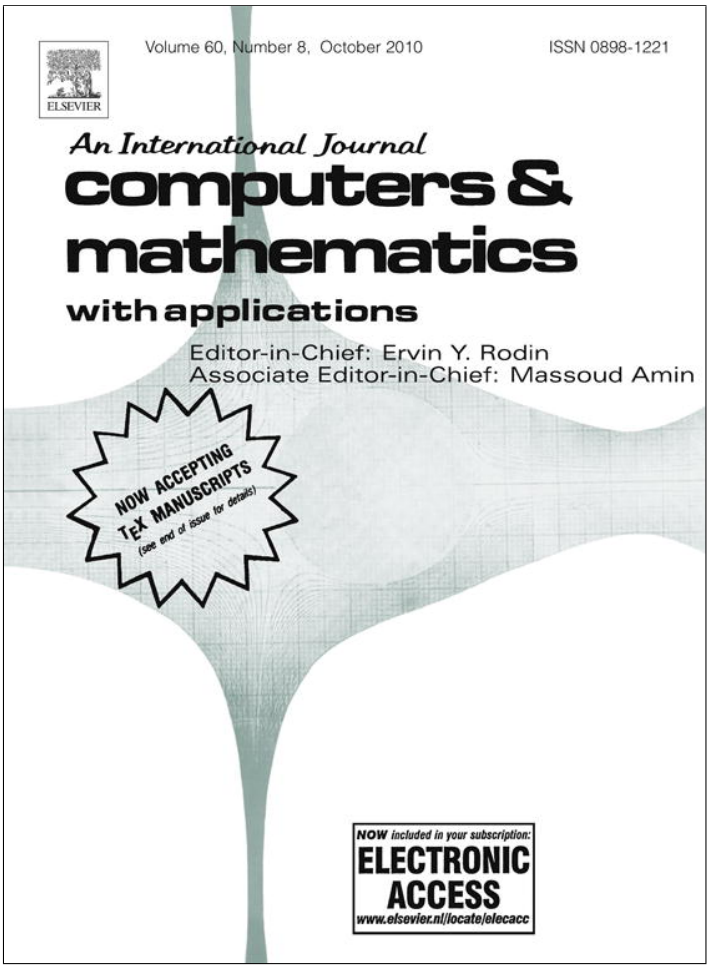

Computers and Mathematics with Applications 60 (2010) 2445–2459

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

Ion transport in inhomogeneous media based on the bipartition model for primary ions

M. Asadzadeh [a,*], A. Brahme [b], J. Kempe [b]

[a] Department of Mathematics, Chalmers University of Technology and Göteborg University, SE–412 96, Göteborg, Sweden

[b] Medical Radiation Physics, Department of Oncology-Pathology, Karolinska Institute, Stockholm, Sweden

ARTICLE INFO

Article history:
Received 7 May 2010
Received in revised form 21 July 2010
Accepted 14 August 2010

Dedicated to the memory of Luo Zheng-Ming

Keywords:
Charged particle transport equation
Ion transport
Inhomogeneous media
Bipartition model

ABSTRACT

The present paper is focused on the mathematical modeling of the charged particle transport in nonuniform media. We study the energy deposition of high energy protons and electrons in an energy range of ≈50–500 MeV. This work is an extension of the bipartition model; for high energy electrons studied by Luo and Brahme in [Z. Luo, A. Brahme, High energy electron transport, Phys. Rev. B 46 (1992) 739–752] [42]; and for light ions studied by Luo and Wang in [Z. Luo, S. Wang, Bipartition model of ion transport: an outline of new range theory for light ions, Phys. Rev. B 36 (1987) 1885–1893]; to the field of *high energy* ions in inhomogeneous media with the retained energy-loss straggling term. In the bipartition model, the transport equation is split into a coupled system of convection–diffusion equations controlled by a partition condition. A similar split is obtained in an asymptotic expansion approach applied to the linear transport equation yielding pencil beam and broad beam models, which are again convection–diffusion type equations. We shall focus on the bipartition model applied for solving three types of problems: (i) normally incident ion transport in a slab; (ii) obliquely incident ion transport in a semi-infinite medium; (iii) energy deposition of ions in a multilayer medium. The broad beam model of the proton absorbed dose was illustrated with the results of a modified Monte Carlo code: *SHIELD - HIT+*.

1. Introduction

Charged particles entering into a medium undergo multiple elastic and inelastic collisions. The elastic collisions that result alter mainly the direction and to a much lesser extent the energy of the particles, whereas the inelastic collisions reduce the energy of the particles but do not generally cause significant change in their directions. In the present paper we, primarily, assume a broad beam of *forward-directed* ions normally incident at the boundary of a semi-infinite medium entering the domain in a direction labeled as the positive direction of the x-axis. As a result of collisions (because of the forward-directed assumption), only, a very small portion of the ions is scattered to *large angles*. Except at very low energies, very few ions will have a directional change beyond a certain minimal angle θ_m, determined by the *bipartition condition*. Above this angle the ions will have a *diffusion-like* transport behavior and with, almost, isotropic angular distribution. Hence, their transport behavior is, preferably, described using P_n-approximations of spherical harmonics. The remaining most significant portion of the ion particles, deflecting slightly ($<\theta_m$) from the original direction, are convective ions and refereed to as *forward-directed* ions. To separate the large-angle scattered and forward-directed ions properly, the bipartition condition is introduced. The current model is based on a split, of the scattering integral (kernel), through adding and

* Corresponding author.
E-mail addresses: mohammad@chalmers.se (M. Asadzadeh), anders.brahme@ki.se (A. Brahme), johanna.kempe@ki.se (J. Kempe).

0898-1221/$ – see front matter © 2010 Elsevier Ltd. All rights reserved.
doi:10.1016/j.camwa.2010.08.040

subtracting the diffusion ion source to the diffusion and straightforward equations, respectively. A similar approach is given through the split of the scattering cross-section into the hard and soft parts, see [1]. This kind of splitting strategy is more common in medical physics studies related to the application of particle beams in cancer therapy. In the bipartition modeling procedure the underlying physics is for the case of ions injected into a background medium with large atomic weight (soft tissue): a transport phenomenon described by assuming a strong algebraic fall-off of the scattering kernel from its peaks at "zero" angle and energy. The underlying partial differential equation is therefore the Boltzmann equation within the Fokker–Planck realm, studied as pencil beam and broad beam models. Alternatively, the particle beam models are derived using asymptotic expansions, see, e.g. [2–5]. Both bipartition and asymptotically derived beam models are classified as *convection-dominated* convection–diffusion equations. In [6] finite element approximations for an asymptotically derived broad beam equation is compared with the results from the bipartition model. For related studies in asymptotically derivations pencil beam equations see, e.g. [1–4,7–10]. Bellomo and co-authors have recently developed and presented a series of mathematical studies in cancer modeling and [11–14]. Further studies concerning transport in biological tissues can be found in [15,16]. For some other related studies see, e.g. in [17,18]. [19] study a method for the semiconductors. Finally, an exposition of connection between kinetic methods and finite difference schemes is given in [20].

The ion transport describing the actual process of energetic ions in absorbing media is formulated for the ion distribution function $f(\mathbf{x}, \mathbf{u}, E)$, also called the *ion fluence differential*, in angle and energy. Here $\mathbf{u} := \mathbf{v}/|\mathbf{v}|$, where $\mathbf{v} \in \mathbb{R}^3 \setminus \{0\}$ is the velocity. Then $f(\mathbf{x}, \mathbf{u}, E)\mathrm{d}\mathbf{u}\mathrm{d}E$ represents the ion fluence at point $\mathbf{x} \in \mathbb{R}^3$, with direction between $\mathbf{u}$ and $\mathbf{u} + \mathrm{d}\mathbf{u}$ and energy between E and $E + \mathrm{d}E$ ($E \in \mathbb{R}^+$). Due to the statistical balance principle we may write the following ion transport equation derived from the transport equation by Lewis and Miller in [21],

$$\mathbf{u} \cdot \nabla_{\mathbf{x}} f - \frac{\partial(\rho f)}{\partial E} = \frac{1}{2}\frac{\partial^2(\Omega f)}{\partial E^2} + N \int_{4\pi} \mathrm{d}\mathbf{u}' \left\{ \left[f(\mathbf{x}, \mathbf{u}', E) - f(\mathbf{x}, \mathbf{u}, E) \right] \times \sigma_n(E', 2E(1 - \mathbf{u} \cdot \mathbf{u}')M_1/M_2) \right\} + S(\mathbf{x}, \mathbf{u}, E), \tag{1.1}$$

where $\rho = \rho_e + \rho_n$ is the total stopping power, with ρ_e being the electronic stopping power and ρ_n the nuclear stopping power. $\Omega = \Omega_c + \Omega_r$ is the total energy-loss straggling factor where Ω_c is the collision energy-loss straggling factor and Ω_r is the radiation energy-loss straggling factor. N is the number of solid atoms in unit volume of the medium, M_1 and M_2 are the atomic weights of the incident ions and the medium, respectively (for slightly heavy ions $M_1 < M_2$, whereas for light ions $M_1 \ll M_2$) and S is the source. Generally, $E' \in \mathbb{R}^+$ and $\mathbf{u}' \in S^2$. We shall study the problem (1.1) for $E' \in [0, E_0]$ and $\mathbf{u}' \in S_0 \subset S^2$. We shall assume a *continuous slowing down approximation* (CSDA) to justify for the collision integral formulated as in (1.1), as well as for the presence of the *energy-loss straggling* term $-\frac{1}{2}\frac{\partial^2(\Omega f)}{\partial E^2}$. In some studies for light ion transport, see [22], this energy-loss straggling term is neglected. Hence, in this setting the terms in the ion transport equation (1.1) are related to three, physically justified, quantities:

(i) the energy-loss straggling term: $-\frac{1}{2}\frac{\partial^2(\Omega f)}{\partial E^2}$,
(ii) the elastic scattering cross-section: σ_n,
(iii) the total stopping power of ions: ρ.

The most specific assumption for the present study is that, following [22] and the references therein, for proton ions, we have assigned an inverse polynomial approximation for the cross-section term in form of separated inverse *power functions* in E and $1 - \mathbf{u} \cdot \mathbf{u}'$. Other forms of radiation interactions are presented, e.g. [23].

Neutral (photon, i.e. X-ray) and charged (electron and ion) particle beams are extensively used in radiation therapy both for early cancer detection and dose computations/algorithms see, e.g. [24–35].

The outline of this paper is as follows: In Section 2 we start with the ion transport equation under the CSDA assumption and derive a computable form of the partition condition and bipartition coefficients. Section 3 is devoted to the bipartition model for the transport of normally incident ions in a semi-infinite medium. Here we derive the key parameters: Legendre coefficients f_{sl} for the distribution function of the straightforward particles, as well as the Legendre coefficients S_l for the diffusion source. Due to the singularity of the kernel, both parameters are derived by approximation in a Fourier transform procedure. We also derive the equation for diffusion ion group and the associated boundary conditions. In Section 4 we extend the bipartition model of Section 3 to obliquely incident ions. In Section 5 we study the energy deposition of ions in a multilayer medium and derive a closed form relation for the *dose* (deposited ion energy) on each layer. Finally, our concluding Section 6 is devoted to some simulation results for the bipartition model using a modified Monte Carlo code.

2. Bipartition model for ion transport under CSDA

To describe the transport of ions of, e.g., ≈50–600 MeV energy, the energy-loss straggling is a significant term that, retained in the study of the bipartition, contributes to the accuracy of the model. We consider an ion beam of energy E_0 normally incident on the hypersurface of a semi-infinite medium. For our physical model we consider a scattering kernel with strong algebraic fall-off behavior from its peaks at zero angle and zero energy. To this end we assume an inverse power function approximation for the elastic cross-section for ion transport, (see also [23]), viz

$$\sigma_n(E, \mathbf{u} \cdot \mathbf{u}') \approx CE^{-2k}(1 - \mathbf{u} \cdot \mathbf{u}')^{-1-k}, \tag{2.1}$$

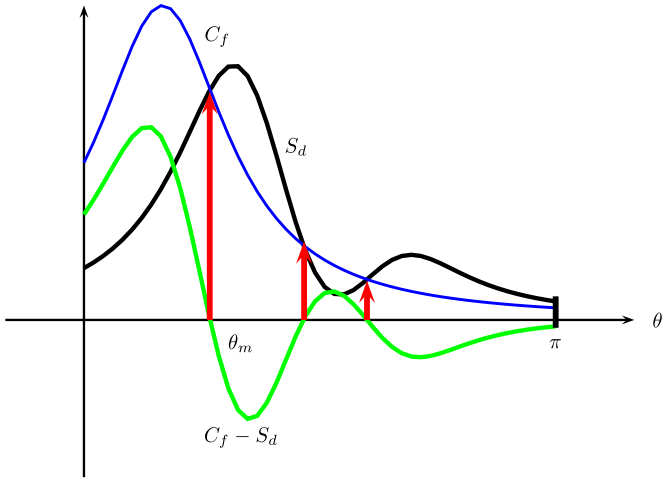

Fig. 1. The extract of diffusion source S_d from the collision term C_f.

where C is a constant depending on E_0, atomic numbers and also Bohr radius (a factor of the classical electron radius, see [22] for details), $k \gg 1$ is a positive integer which corresponds to the magnitude of the algebraic fall-offs. Further, we let the outward normal to the semi-infinite region on the left to be along the positive x-axis inside the solid, then using the standard vector notation: $\mathbf{x} = (x, y, z)$, the high energy ion/electron transport equation under the CSDA is given by (see [32]),

$$-\frac{\partial(\rho f)}{\partial E} + \mu\frac{\partial f}{\partial x} - \frac{1}{2}\frac{\partial^2(\Omega f)}{\partial E^2} := \tilde{\delta} + C_f \equiv \frac{1}{2\pi}\delta(x)\delta(E - E_0)\delta(1-\mu) + CE^{-2k}\int_{4\pi} \mathrm{d}\mathbf{u}'[f(x,\mu',E) - f(x,\mu,E)] \times (1 - \mathbf{u}\cdot\mathbf{u}')^{-k-1}, \tag{2.2}$$

where μ is the cosine of the angle between the direction of the ions and the x-axis. C_f is called the scattering integral and represents the net increase in the number of particles per unit solid angle $\mathbf{u}$, passing through a unit distance, caused by elastic scattering. From (2.2) and the property that the small-angle elastic scattering of ions is dominating, the main feature of C_f can be shown as in Fig. 1.

In the bipartition strategy the scattering integral is divided into two parts, of which one is the comparatively isotropic diffusion ion source S_d, including almost all of the "large-angle" scattered ions, the other is the remaining part that spreads mainly in the forward, small-angle, direction.

To solve for spherical harmonic coefficients, using Fourier transformation in E would reduce the equation to an ODE in x, where the presence of (2.1) would enforce yet another approximation in computing Fourier integrals. This is specified by (3.7) and outlined in Remark 3.2. For a more general approach see, e.g. [36].

The bipartition model splits f into two parts:

$$f(x,\mu,E) = f_s(x,\mu,E) + f_d(x,\mu,E), \tag{2.3}$$

where f_s is the forward-directed ion distribution satisfying

$$-\frac{\partial(\rho f_s)}{\partial E} + \mu\frac{\partial f_s}{\partial x} - \frac{1}{2}\frac{\partial^2(\Omega f_s)}{\partial E^2} = -S_d + \frac{1}{2\pi}\delta(x)\delta(E - E_0)\delta(1-\mu) + CE^{-2k}\int_{4\pi} \mathrm{d}\mathbf{u}'[f_s(\mathbf{x},\mu',E) - f_s(x,\mu,E)] \times (1 - \mathbf{u}\cdot\mathbf{u}')^{-k-1}, \tag{2.4}$$

and f_d is the distribution of the diffusion ion particles satisfying

$$-\frac{\partial(\rho f_d)}{\partial E} + \mu\frac{\partial f_d}{\partial x} - \frac{1}{2}\frac{\partial^2(\Omega f_d)}{\partial E^2} = S_d + CE^{-2k}\int_{4\pi} \mathrm{d}\mathbf{u}'[f_d(\mathbf{x},\mu',E) - f_d(x,\mu,E)] \times (1 - \mathbf{u}\cdot\mathbf{u}')^{-k-1}. \tag{2.5}$$

In the bipartition model we deduct the large-angle scattering source from the collision term in the straightforward equation (2.2) by means of subtracting $S_d(x,\mu,E)$. Consequently in (2.4), the scattering process generating large-angle ions is removed from the forward-directed (2.2). Then, *the partition condition* is given by

$$S_d(x,\mu_i,E) = C_{f_s}(x,\mu_i,E), \quad i = 0, 1, \ldots, m. \tag{2.6}$$

The condition (2.6) means that all the large-angle scattered ions in the straightforward ion group are regarded as the secondary diffusion ion source S_d. *To define the bipartition condition, we require that the intensity of this diffusion ion source*

at the $m+1$ large-angle directions to be exactly equal to the values of collision integral at the same directions. We expand the distribution functions f_s and f_d and the diffusion source S_d into Legendre polynomials,

$$f_s(x,\mu,E)=\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\mu)f_{sl}(x,E), \tag{2.7}$$

$$f_d(x,\mu,E)=\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\mu)f_{dl}(x,E), \tag{2.8}$$

$$S_d(x,\mu,E)=\sum_{l=0}^{m}\frac{2l+1}{4\pi}P_l(\mu)S_{dl}(x,E). \tag{2.9}$$

The collision integral for f_s, forward-directed particles, can then be computed as

$$C_{f_s}(x,\mu,E)=-CE^{-2k}\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}\eta_l P_l(\mu)f_{sl}(x,E), \tag{2.10}$$

where

$$\eta_l=2\pi\int_{-1}^{1}[1-P_l(\mu)](1-\mu)^{-1-k}\mathrm{d}\mu. \tag{2.11}$$

Obviously $\eta_0=0$ and for $l\geq 1$, η_l is obtained from the following recursive formula (see [22]),

$$(l+1-k)\eta_{l+1}=(l+1+k)\eta_l+4\pi/2^k,\quad \eta_0=0. \tag{2.12}$$

Inserting (2.10) into (2.6) and using (2.9) we get the specific partition condition:

$$-CE^{-2k}\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}\eta_l P_l(\mu_i)f_{sl}(x,E)=\sum_{l=0}^{m}\frac{2l+1}{4\pi}P_l(\mu_i)S_{dl}(x,E). \tag{2.13}$$

Therefore

$$S_{dl}(x,E)=-CE^{-2k}\left(\eta_l f_{sl}(x,E)+\sum_{l'=k+1}^{\infty}\eta_l' D_{ll'}f_{sl'}(x,E)\right). \tag{2.14}$$

The bipartition coefficient $D_{ll'}$ is given by

$$D_{ll'}=\frac{2l'+1}{2l+1}\cdot\frac{\Delta_{ll'}}{\Delta_l}, \tag{2.15}$$

where we have used Cramer's rule with

$$\Delta_l=det[\mathbf{P}_0(\mu),\mathbf{P}_1(\mu),\ldots,\mathbf{P}_l(\mu),\ldots,\mathbf{P}_m(\mu)],$$
$$\Delta_{ll'}=det[\mathbf{P}_0(\mu),\mathbf{P}_1(\mu),\ldots,\mathbf{P}_{l'}(\mu),\ldots,\mathbf{P}_m(\mu)],$$

where

$$\mathbf{P}_j(\mu)=[P_j(\mu_0),P_j(\mu_1),\ldots,P_j(\mu_m)]^T,\quad j=0,1,\ldots,m.$$

For further discussions on *small-angle condition* and other quantities, see [32–34].

3. The primary ion transport including energy-loss straggling

3.1. The straightforward ion group

To compute the distribution function f_s for convective ions group we shall assume that the following properties hold:

(p1) The bipartition condition: $C_f(x,\mu_i,E)=S_d(x,\mu_i,E)$, $i=0,1,\ldots,m$,
(p2) The narrow energy spectrum approximation (NESA),
(p3) The small-angle approximation (SAA).

The idea of NESA is that: *"if the width of energy spectrum for a charged particle beam is much narrower than the average energy of the beam, then the interaction cross-section between the particles in the beam and the atoms in medium in an integral, weighted*

with the charged particle spectrum, can be replaced by its truncated Taylor series around the average energy". The small-angle approximation, SAA is to substitute μ in the term $\mu(\partial f_s/\partial x)$ by $\mu_a(x)$; an average direction cosine

$$\mu_a(x) = \frac{\int_0^{E_0}\int_{-1}^{1}\mu f_s(x,\mu,E)\mathrm{d}\mu\mathrm{d}E}{\int_0^{E_0}\int_{-1}^{1} f_s(x,\mu,E)\mathrm{d}\mu\mathrm{d}E} = \frac{\int_0^{E_0} f_{s1}(x,E)\mathrm{d}E}{\int_0^{E_0} f_{s0}(x,E)\mathrm{d}E}. \tag{3.1}$$

Remark 3.1. In the presence of the energy-loss straggling term: $-\frac{1}{2}\frac{\partial^2(\Omega f)}{\partial E^2}$, the SAA is given by (3.1). Consequently, to transfer the equation for f_s to an ordinary differential equation, the suitable Fourier transform variable is E. Neglecting the energy-loss straggling term, the SAA may be characterized by defining $\mu_a(E)$ through replacing the integrations over E in (3.1) by integrations over x and then perform Fourier transformation in x.

To proceed, for convective ion particles arriving at point x, we introduce the average path-length $L_a(x)$ and the corresponding average energy $E_a(x)$, by

$$L_a(x) = \int_0^x \frac{1}{\mu_a(x')}\mathrm{d}x', \tag{3.2}$$

$$E_a(x) = E_0 - \int_0^{L_a} L(E, E_0 - E')\mathrm{d}E', \tag{3.3}$$

where $L(E, E_0 - E')$ is an approximation of the conventional stopping power ρ. In this way, using (2.7)–(2.11), (2.14) and (3.1)–(3.3), in integrating (2.4) with respect to μ, we end up with the equation for the Legendre coefficients f_{sl} as

$$\begin{aligned}\mathcal{T} f_{sl} &:= -\frac{\partial}{\partial E}\left[L(E,E')f_{sl}(x,E)\right] + \mu_a(x)\frac{\partial f_{sl}}{\partial x} - \frac{1}{2}\frac{\partial^2}{\partial E^2}\left[\Omega_c f_{sl}(x,E)\right]\\ &= -CE^{-2k}\sum_{l'=m+1}^{\infty}\eta_{l'}D_{ll'}f_{sl'}(x,E) + \delta(x)\delta(E-E_0); \quad l \le m,\end{aligned} \tag{3.4}$$

$$\mathcal{T} f_{sl} := -CE^{-2k}\eta_l f_{sl}(x,E) + \delta(x)\delta(E-E_0); \quad l > m, \tag{3.5}$$

where $\mathcal{T}$ is a *degenerate (no second derivative in x) convection–diffusion operator*

$$\mathcal{T}\bullet = \left(-\frac{\partial}{\partial E}L(E,E') + \mu_a(x)\frac{\partial}{\partial x} - \frac{1}{2}\frac{\partial^2}{\partial E^2}\Omega_c\right)\bullet.$$

By some formal calculus, one can show that

$$f_{sl}(x,E) = -\sum_{l'=m+1}^{\infty} D_{ll'}f_{sl'}(x,E), \quad l \le m. \tag{3.6}$$

Therefore, as soon as, we obtain a solution of (3.5), we automatically have a solution for (3.4) as well. To solve (3.5) it is natural to transfer the equation to an ODE in x by imposing Fourier transformation in E. This, however, is prohibited due to singularity of E^{-2k}, $(k > 0)$ in the Fourier domain. A remedy would be through using the notion of average energy $E_a(x)$ (>0) introduced in (3.3) and NESA approximation for weighted Fourier transform viz;

$$\mathcal{F}\left[w(E)f_{sl}(E)\right](\xi) = \int_{-\infty}^{\infty}\mathrm{e}^{-\mathrm{i}\xi E}w(E)f_{sl}(E)\mathrm{d}E \approx w(E_a)\hat{f}_{sl}(\xi), \tag{3.7}$$

where

$$\hat{f}_{sl}(x,\xi) = \int_{-\infty}^{\infty}\mathrm{e}^{-\mathrm{i}\xi E}f_{sl}(x,E)\mathrm{d}\xi, \tag{3.8}$$

is the Fourier transform of $f_{sl}(x,E)$ with respect to E and $w(E) := w(x,E)$ is any sufficiently smooth weight function (e.g. interaction function between ions and the background atoms).

Remark 3.2. Generally, to justify an approximation of the form (3.7), in a Fourier transform, E_a should be chosen so that

$$w(x,E_a) \approx \hat{w}(x,0) = \int_{-\infty}^{\infty} w(x,E)\mathrm{d}E. \tag{3.9}$$

Since for $\hat{w}(x,\xi) = \int_{-\infty}^{\infty}\mathrm{e}^{-\mathrm{i}x\xi}w(x,E)\mathrm{d}E$, the Fourier transform of $w(x,E)$, we have

$$\mathcal{F}\left[w(x,E)f_{sl}(x,E)\right](\xi) = \hat{w}(x,\xi) *_\xi \hat{f}_{sl}(x,\xi), \tag{3.10}$$

we may write

$$w(x,E)=\frac{w(x,E)}{w(x,E_a)}w(x,E_a):=g(x,E)w(x,E_a), \tag{3.11}$$

where, due to (3.9), $\int_{-\infty}^{\infty} g(x,E)\mathrm{d}E\approx 1$, i.e. $g\in L_1$. Now, since

$$\hat{w}(x,\xi)=w(x,E_a)\hat{g}(x,\xi), \tag{3.12}$$

hence,

$$\hat{w}(x,\xi)*_\xi \hat{f}_{sl}(x,\xi)=w(x,E_a)\hat{g}(x,\xi)*_\xi \hat{f}_{sl}(x,\xi), \tag{3.13}$$

and under certain assumption (if, e.g. $g(x,E)\approx\delta_x(E)$, see Folland [37], chapter 7) we may choose an approximation of the form:

$$\hat{g}(x,\xi)*_\xi \hat{f}_{sl}(x,\xi)\approx\hat{f}_{sl}(x,\xi).$$

Our goal is to give a closed form approximation for $\hat{f}_{sl}$. Then, by the inverse Fourier transform we can get the lth Legendre components f_{sl}. To this approach it suffices to invoke the following approximation of the weight function:

$$w(x,E)=\frac{w(x,E)}{w(x,E_a)}w(x,E_a)\approx\delta(E)w(E_a,x), \tag{3.14}$$

i.e., we approximate $g:=w/w_a$ by the Dirac δ function in energy variable. Hence

$$\mathcal{F}\left[w(E,x)f_{sl}(x,E)\right](\xi)\approx w(x,E_a)\left(\hat{\delta}(\xi)*\hat{f}_{sl}(x,\xi)\right)=w(x,E_a)\hat{f}_{sl}(x,\xi). \tag{3.15}$$

This however is *too involved*: in reality the energy variable ranges in an interval $I=[0_-,E_0]$ (0_-, to avoid 0 as starting limit for the integration of $\delta(E)$ over $[0,E_0]$) and one may just use the *integral form of the generalized mean value theorem*:

Lemma 3.3. *If f and g are continuous on the interval $[a,b]$ and f does not change sign on that interval, then there exists a point $p\in[a,b]$ such that*

$$\int_a^b f(x)g(x)\mathrm{d}x=g(p)\int_a^b f(x)\mathrm{d}x. \tag{3.16}$$

Hence the indefinite integral in (3.7) can be replaced by an integral over $I=[0_-,E_0]$ and, assuming that f_{sl} is positive for all l, the mean value theorem above would provide us with an equality (instead of approximation (3.15)) in (3.7). Thus, with some physically motivated manipulations, the Fourier transform of (3.5), with respect to E yields the approximate equation

$$-(\mathrm{i}\xi)\left[L(E_a,\Delta)\hat{f}_{sl}(x,\xi)\right]+\mu_a(x)\frac{\partial\hat{f}_{sl}(x,\xi)}{\partial x}-\frac{(\mathrm{i}\xi)^2}{2}\Omega_c(E_a)\hat{f}_{sl}(x,\xi)=-CE_a^{-2k}\eta_l\hat{f}_{sl}(x,\xi)+\delta(x)\mathrm{e}^{-\mathrm{i}\xi E_0}, \tag{3.17}$$

i.e.,

$$\left[CE_a^{-2k}\eta_l-(\mathrm{i}\xi)L(E_a,\Delta)+\frac{\xi^2}{2}\Omega_c(E_a)\right]\hat{f}_{sl}(x,\xi)+\mu_a(x)\frac{\partial\hat{f}_{sl}(x,\xi)}{\partial x}=\delta(x)\mathrm{e}^{-\mathrm{i}\xi E_0},$$

where $\Delta:=E_0-E'$. To simplify we write this relation as

$$\lambda(E_a,\xi)\hat{f}_{sl}(x,\xi)+\mu_a(x)\frac{\partial\hat{f}_{sl}(x,\xi)}{\partial x}=\delta(x)\mathrm{e}^{-\mathrm{i}\xi E_0}, \tag{3.18}$$

or equivalently

$$\frac{\partial\hat{f}_{sl}(x,\xi)}{\partial x}+\frac{\lambda(E_a,\xi)}{\mu_a(x)}\hat{f}_{sl}(x,\xi)=\frac{1}{\mu_a(x)}\delta(x)\mathrm{e}^{-\mathrm{i}\xi E_0}. \tag{3.19}$$

Let now $\Lambda(x)=\int\frac{\lambda(E_a,\xi)}{\mu_a(x)}\mathrm{d}x=\lambda(E_a,\xi)\int\frac{1}{\mu_a(x)}\mathrm{d}x$, or $\Lambda(x)=\lambda(E_a,\xi)\int_0^x\frac{1}{\mu_a(x')}\mathrm{d}x':=\lambda(E_a,\xi)L_a(x)$, and multiply (3.19) by the integrating factor $\mathrm{e}^{\Lambda(x)}$ to get

$$\mathrm{e}^{\Lambda(x)}\frac{\partial\hat{f}_{sl}(x,\xi)}{\partial x}+\mathrm{e}^{\Lambda(x)}\frac{\lambda(E_a,\xi)}{\mu_a(x)}\hat{f}_{sl}(x,\xi)=\mathrm{e}^{\Lambda(x)}\frac{1}{\mu_a(x)}\delta(x)\mathrm{e}^{-\mathrm{i}\xi E_0}, \tag{3.20}$$

i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[\mathrm{e}^{\Lambda(x)}\hat{f}_{sl}(x,\xi)\right]=\frac{1}{\mu_a(x)}\mathrm{e}^{\Lambda(x)}\delta(x)\mathrm{e}^{-\mathrm{i}\xi E_0}, \tag{3.21}$$

which, integrating over $(0, x)$ yields

$$\mathrm{e}^{\Lambda(x)}\hat{f}_{sl}(x,\xi)-\mathrm{e}^{\Lambda(0)}\hat{f}_{sl}(0,\xi)=\frac{1}{\mu_a(0)}\mathrm{e}^{\Lambda(0)}\mathrm{e}^{-\mathrm{i}\xi E_0}. \tag{3.22}$$

Recall that, starting with the straightforward, incident, ions at $x = 0$; $\mu_a(0) \approx 1$, and consequently we may write

$$\hat{f}_{sl}(x,\xi)\approx \mathrm{e}^{-(\Lambda(x)-\Lambda(0))}\left(\hat{f}_{sl}(0,\xi)+\mathrm{e}^{-\mathrm{i}\xi E_0}\right),\quad x\neq 0. \tag{3.23}$$

Note that

$$\begin{aligned}\Lambda(x) &= C\eta_l\int_0^x\frac{E_a^{-2k}}{\mu_a(x')}\mathrm{d}x'-\mathrm{i}\xi\int_0^x\frac{L[E_a(x'),\Delta]}{\mu_a(x')}\mathrm{d}x'+\frac{1}{2}\xi^2\int_0^x\frac{\Omega_c[E_a(x')]}{\mu_a(x')}\mathrm{d}x'\\ &:= C\eta_l q(x)-\mathrm{i}\xi\Delta E(x)+\xi^2\omega(x),\end{aligned}$$

and $q(0) = \Delta E(0) = \omega(0) = 0$, i.e. $\Lambda(0) = 0$. Further, by the forward-directed assumption and with no back-scattering to the left of $x = 0$ we get

$$f_{sl}(x,E)=\hat{f}_{sl}(x,\xi)=0,\quad \text{for } x<0.$$

Hence

$$\hat{f}_{sl}(x,\xi)=\begin{cases}\mathrm{e}^{-\mathrm{i}\xi(E_0-\Delta E(x))-C\eta_l q(x)-\xi^2\omega(x)}, & x>0,\\ 0 & x<0.\end{cases} \tag{3.24}$$

Thus, we have

$$f_{sl}(x,\xi)=\frac{1}{2\pi}\mathrm{e}^{-C\eta_l q(x)}\int_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}\xi E}\cdot\mathrm{e}^{-\mathrm{i}\xi(E_0-\Delta E(x))}\cdot\mathrm{e}^{-\xi^2\omega(x)}\mathrm{d}\xi. \tag{3.25}$$

We define

$$\mathcal{G}(x,E):=\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}\xi E}\cdot\mathrm{e}^{-\mathrm{i}\xi(E_0-\Delta E(x))}\cdot\mathrm{e}^{-\xi^2\omega(x)}\mathrm{d}\xi. \tag{3.26}$$

Comparing with the inverse Fourier transform

$$\mathcal{G}(x,E)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}\xi E}[\hat{\mathcal{G}}(x,\xi)](E)\mathrm{d}\xi, \tag{3.27}$$

we have that

$$\left[\hat{\mathcal{G}}(x,\xi)\right](E_0-\Delta E(x))=\begin{cases}\mathrm{e}^{-\mathrm{i}\xi(E_0-\Delta E(x))-\xi^2\omega(x)}, & x\geq 0,\\ 0 & x<0.\end{cases} \tag{3.28}$$

Now by the symmetry relation for the Fourier transform for the Gaussian:

$$\hat{h}(x,\xi)=\mathrm{e}^{-\xi^2\omega(x)}\Longrightarrow h(x,E)=\frac{1}{2\sqrt{\pi\omega(x)}}\mathrm{e}^{-\frac{E^2}{4\omega(x)}} \tag{3.29}$$

and with $E_a = E_0 - \Delta E$, using the inverse Fourier transform, we may write

$$\mathcal{G}(x,E)=h(x,E-E_a)=\frac{1}{2\pi}\sqrt{\frac{\pi}{\omega(x)}}\mathrm{e}^{-\frac{(E-E_a)^2}{4\omega(x)}}, \tag{3.30}$$

so that finally we get

$$f_{sl}(x,E)=\frac{1}{2\pi}\sqrt{\frac{\pi}{\omega(x)}}\mathrm{e}^{-(E-E_a)^2/4\omega(x)}\cdot\mathrm{e}^{-C\eta_l q(x)}. \tag{3.31}$$

Thus, recalling (3.4) and (3.5), the Legendre coefficients for the distribution function f_{sl} can be written as

$$f_{sl}(x,E)=\frac{1}{2\pi}\sqrt{\frac{\pi}{\omega(x)}}\mathrm{e}^{-(E-E_a)^2/4\omega(x)}\gamma_l(x) \tag{3.32}$$

where

$$\gamma_l(x) = \begin{cases} -\sum_{l'=m+1}^{\infty} D_{ll'} \mathrm{e}^{-C\eta_{l'} q(x)}, & l \le m, \\ \mathrm{e}^{-C\eta_l q(x)}, & l > m. \end{cases} \tag{3.33}$$

As in the case of (3.5) and (3.4), once we compute γ_l for $l > m$, then we get automatically the sum in (3.33). Thus γ_l is easily computable, recalling that

$$q(x) = \int_0^x \frac{E_a(x')^{-2k}}{\mu_a(x')} \mathrm{d}x', \qquad \Delta E(x) = \int_0^x \frac{L[E_a(x'), \Delta]}{\mu_a(x')} \mathrm{d}x', \quad \text{and} \quad \omega(x) = \frac{1}{2} \int_0^x \frac{\Omega_c[E_a(x')]}{\mu_a(x')} \mathrm{d}x'. \tag{3.34}$$

Having computed f_{sl}, we can give a, numerically, computable expression for $S_l(x, E)$ in (2.14) and prepare for the study of the diffusion ion group.

Proposition 3.4. *For the bipartition model the Legendre coefficients $S_{dl}(x, E)$ for the diffusion source term in (2.14) are given by*

$$S_{dl}(x, E) = \left[-CE^{-2k} \eta_l + \frac{\mathrm{d}}{\mathrm{d}x} \ln(\gamma_l(x)) \right] f_{sl}(x, E). \tag{3.35}$$

Proof. Differentiating (3.32) we have

$$\frac{\partial f_{sl}}{\partial E} = \left[-\frac{E - E_a}{2\omega} \right] f_{sl}, \tag{3.36}$$

and

$$\begin{aligned} \frac{\partial^2 f_{sl}}{\partial E^2} &= -\frac{1}{2\omega} f_{sl} - \frac{E - E_a}{2\omega} \frac{\partial f_{sl}}{\partial E} = -\frac{1}{2\omega} f_{sl} - \left(\frac{E - E_a}{2\omega} \right) \left[-\frac{E - E_a}{2\omega} \right] f_{sl} \\ &= \left[\frac{(E - E_a)^2 - 2\omega}{4\omega^2} \right] f_{sl}. \end{aligned} \tag{3.37}$$

Further

$$\begin{aligned} \frac{\partial f_{sl}}{\partial x} &= \frac{1}{2\pi} \cdot \sqrt{\pi} \left(-\frac{1}{2} \omega^{-3/2} \right) \cdot \mathrm{e}^{-(E-E_a)^2/(4\omega(x))} \gamma_l(x) \\ &\quad + \frac{1}{2\pi} \sqrt{\frac{\pi}{\omega}} \mathrm{e}^{-(E-E_a)^2/(4\omega(x))} \left(-\frac{2(E - E_a)}{4\omega(x)} \cdot \frac{\mathrm{d}E_a}{\mathrm{d}x} - \frac{(E - E_a)^2}{4} \cdot \frac{-1}{\omega^2} \frac{\mathrm{d}\omega}{\mathrm{d}x} \right) \gamma_l(x) \\ &\quad + \frac{1}{2\pi} \sqrt{\frac{\pi}{\omega}} \mathrm{e}^{-(E-E_a)^2/(4\omega(x))} \frac{\mathrm{d}}{\mathrm{d}x} \gamma_l(x) \\ &= \left[-\frac{1}{2\omega} \frac{\mathrm{d}\omega}{\mathrm{d}x} - \frac{E - E_a}{2\omega} \frac{\mathrm{d}E_a}{\mathrm{d}x} + \frac{(E - E_a)^2}{4\omega^2} \frac{\mathrm{d}\omega}{\mathrm{d}x} + \frac{\mathrm{d}}{\mathrm{d}x} (\ln \gamma(x)) \right] f_{sl}, \end{aligned}$$

where, for the logarithmic term, we have used the identity $\gamma_l'(x) = \frac{\gamma_l'}{\gamma_l} \gamma_l$. Inserting these derivatives in (3.4) and invoking the average quantities defined for the coefficients, and the auxiliary relations

$$\frac{\mathrm{d}\omega}{\mathrm{d}x} = \frac{\Omega_c}{2\mu_a}, \qquad \frac{\mathrm{d}E_a}{\mathrm{d}x} = \frac{l}{\mu_a}, \tag{3.38}$$

yields

$$-CE^{-2k} \sum_{l'=m+1}^{\infty} \eta_{l'} D_{ll'} f_{sl'}(x, E) + \delta(x)\delta(E - E_0) = f_{sl}(x, E) \frac{\mathrm{d}}{\mathrm{d}x} (\ln \gamma(x)). \tag{3.39}$$

Hence, the Legendre coefficients S_l for the diffusion source term can be written as

$$S_{dl}(x, E) = \left[-CE^{-2k} \eta_l + \frac{\mathrm{d}}{\mathrm{d}x} \ln(\gamma_l(x)) \right] f_{sl}(x, E), \tag{3.40}$$

which is the desired result and the proof is complete. □

3.2. The diffusion ion group

With the diffusion coefficients S_{dl} for the ion source given by (3.40), we can now calculate the Legendre coefficients f_{dl} for the distribution function f_d of the diffusion ions. Due to a nearly isotropic behavior of the angular distribution of diffusion ions, the spherical harmonic moments cannot be decoupled. To circumvent such obstacle a cutoff method, based on P_n-approximation, is commonly used assuming

$$f_{dl}(x, E) = 0, \quad \text{for } l > n. \tag{3.41}$$

Then, a weighted central differencing, see [22,33] for details, yields

$$\begin{aligned} &-\frac{\partial(\rho f_{dl})}{\partial E} + \frac{1}{2l+1}\left[(l+1)\frac{\partial(\mu_a f_{d,l+1})}{\partial x} + l\frac{\partial(\mu_a f_{d,l-1})}{\partial x}\right] - \frac{1}{2}\frac{\partial^2(\Omega f_{dl})}{\partial E^2} \\ &= -CE^{-2k}\eta_l f_{dl} + \tilde{S}_l(x, E), \quad l = 0, 1, \ldots, n, \end{aligned} \tag{3.42}$$

where $f_{d,-1} \equiv 0$ and

$$\tilde{S}_l(x, E) := f_{sl}(x, E)\frac{\mathrm{d}}{\mathrm{d}x}\ln(\gamma_l(x)), \quad l = 0, 1, \ldots, n. \tag{3.43}$$

Under certain assumptions on the coefficients, this set of equations may have closed form analytic solutions. But, in the real applications, the coefficients are rather involved and therefore numerical methods are the most realistic approaches. In this regard, a direct approach to (3.42) and (3.43) is based on a Lax–Wendroff scheme applied to a symmetrical form of (3.42) for the auxiliary function

$$\tilde{f}_{dl}(x, E) := \frac{1}{\sqrt{2l+1}} f_{dl}(x, E). \tag{3.44}$$

Then, $\tilde{f}_{dl}$ would satisfy the following, second order accurate, scheme:

$$\begin{aligned} -\frac{\partial(\rho\tilde{f}_{dl})}{\partial E} &= -\frac{1}{\sqrt{2l+1}}\left[\frac{l+1}{\sqrt{2l+3}}\frac{\partial(\mu_a\tilde{f}_{d,l+1})}{\partial x} + \frac{l}{\sqrt{2l-1}}\frac{\partial(\mu_a\tilde{f}_{d,l-1})}{\partial x}\right] \\ &\quad - \frac{1}{2}\frac{\partial^2(\Omega\tilde{f}_{dl})}{\partial E^2} - CE^{-2k}\eta_l\tilde{f}_{dl} + \frac{1}{\sqrt{2l+1}}\tilde{S}_l, \quad l = 0, 1, \ldots, n. \end{aligned} \tag{3.45}$$

Another interesting scheme is obtained using a finite element approximation applied directly to the diffusion equation

$$-\frac{\partial(\rho f_{dl})}{\partial E} + \mu_a\frac{\partial f_{dl}}{\partial x} - \frac{1}{2}\frac{\partial^2(\Omega f_{dl})}{\partial E^2} = S_{dl}. \tag{3.46}$$

The Eq. (3.46) is a degenerate type convection–diffusion equation which is studied extensively in [7–10], using the *Streamline diffusion* finite element method.

3.3. Boundary conditions

As expecting, for the forward-directed incident ions, only the ions reflected from the solid surface to the left-hand side of the domain may exist at the boundary $x = 0$. Therefore it is reasonable to assume a boundary condition, equivalent to assuming a vacuum medium on the left, of the form,

$$f_d(0, \mu, E) = 0, \quad \mu \geq 0. \tag{3.47}$$

To determine the approximate distribution function for diffusion ions, based on P_n-approximation, we need certain variants of (3.47) formulated for finite number of angular cosines μ. In this regard there are two classical type of discrete boundary conditions proposed by Mark [38] and Marshak [39]. Both conditions are assuming an odd number of discrete cosine directions n. The Mark condition is based on treating the left-hand side as a vacuum of a scape black-box, i.e.,

$$f_d(0, \mu_i, E) = 0, \qquad P_{n+1}(\mu_i) = 0, \quad \mu_i \geq 0,\ i = 1, 2, \ldots, \frac{n+1}{2}. \tag{3.48}$$

The Marshak condition is formulated for the current; ensuring that no diffusion ion current is incident upon the solid surface from the assumed vacuum part:

$$\int_0^1 f_d(0, \mu_i, E)\mu^{2j-1}\mathrm{d}\mu = 0, \quad i = 1, 2, \ldots, \frac{n+1}{2}. \tag{3.49}$$

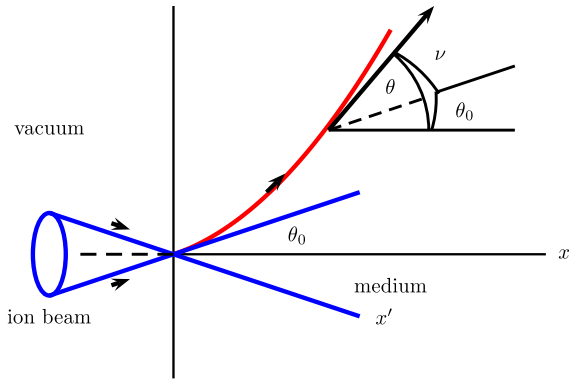

Fig. 2. Obliquely incident ions.

Mark condition is used for higher degree approximations (e.g., for $n > 5$). As the $(n+1)/2$ boundary conditions (3.48) or (3.49) are insufficient to determine $(n+1)$ spherical harmonic moments $\tilde{f}_{dl}$ involved in the Eq. (3.45), additional conditions are supplied for $\mu < 0$. These are of the form

$$\begin{aligned} &\frac{\partial(\rho f_d)}{\partial E} + \frac{1}{2}\frac{\partial^2(\Omega f_d)}{\partial E^2} = \mu_i \frac{\partial(f_d)}{\partial x} + \frac{C}{4\pi}E^{-2k}\sum_{l=0}^{n}(2l+1)\eta_l P_l(\mu_i) f_{dl}(0,E), \\ &P_{n+1}(\mu_i) = 0, \quad \mu_i < 0,\ i = \frac{n+3}{2}, \ldots, n+1 \end{aligned} \tag{3.50}$$

and are described in [22] and the references therein. With the complete set of boundary conditions we are prepared to expand the study to the multilayer case.

4. Obliquely incident ion transport in semi-infinite media

Assume that a conical ion beam of initial energy E_0 is incident upon a semi-infinite homogeneous medium at an incident angle θ_0, as shown in Fig. 2.

The forward peakedness condition for ions is then

$$\frac{\pi}{2} - \theta_0 > \theta_m, \tag{4.1}$$

and therefore there is no influence from the boundary to the distribution function of forward-peaked ions. Even for $\frac{\pi}{2} - \theta_0 < \theta_{min}$, the amount of forward-peaked ions that leave the surface directly is negligible. Thus we neglect the influence of the boundary on the distribution function of convective particles. To proceed we make a coordinate transformation: $(E, \mu, x) \to (E', \nu, x')$, where x and x' are directions of inward normal to the surface and obliquely incident ions, respectively, $\nu = \theta - \theta_0$ is the deflection angle and E' is the energy of oblique ions. Thus, $E' = E$ and $x' = x/\cos\theta$. In this way we can derive the distribution function for the forward-peaked ions of oblique incidence from the distribution function for forward-peaked ions of normal incidence. One may address this as the fact that in the coordinate system (E', ν, x') the distribution function of the forward-peaked ions would remain unchanged. We denote the forward-peaked distribution function and the diffusion ion source in the new coordinate system by $\tilde{f}_s$ and $\tilde{S}_d$, respectively. Then by the above motivation and our result for the normally incident ions we conclude that

$$\tilde{f}_s(x', \nu, E') = \frac{1}{2\pi}\left[\frac{\pi}{\omega}\right]^{1/2} \mathrm{e}^{-(E'-E_a)^2/4\omega(x)} \times \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\cos\nu)\gamma_l(x'), \tag{4.2}$$

and

$$\tilde{S}_d(x', \nu, E') = \frac{1}{2\pi}\left[\frac{\pi}{\omega}\right]^{1/2} \mathrm{e}^{-(E'-E_a)^2/4\omega(x)} \times \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\cos\nu)S_l(x'). \tag{4.3}$$

Now we may return to the original coordinate system, recalling

$$\left\{x' = x/\cos\theta, E' = E, \cos\nu = \cos\theta_0\cos\theta + \sin\theta_0\sin\theta\cos(\varphi - \varphi_0)\right\}. \tag{4.4}$$

Since the cone is symmetric in the azimuthal angle φ, the distribution function of forward-peaked ions, in the original coordinates, should be averaged over φ, i.e.,

$$f_s(x, \mu, E) = \frac{1}{2\pi}\int_0^{2\pi}\tilde{f}_s(x', \cos\nu, E')\mathrm{d}\varphi = \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\cos\theta)f_{sl}(x, E). \tag{4.5}$$

The average projection distance of the forward-peaked ions along the x'-axis is:

$$x' = \int_0^{r'} \mu_a(r')\mathrm{d}r' = \int_0^{r'} \frac{\gamma_1(r')}{\gamma_0(r')}\mathrm{d}r'. \tag{4.6}$$

Thus

$$f_s(x,\mu,E) = \frac{1}{2\pi}\left[\frac{\pi}{\omega}\right]^{1/2} \mathrm{e}^{-(E-E_a)^2/4\omega(x)} \sum_{l=0}^{\infty} \frac{2l+1}{4\pi}\gamma_l(x') \cdot \frac{1}{2\pi}\int_0^{2\pi} P_l(\cos\nu)\mathrm{d}\varphi. \tag{4.7}$$

Using the *addition theorem for Legendre polynomials*, see [40], we have

$$f_{sl}(x,E) = \frac{1}{\sqrt{4\pi\omega(x)}}\mathrm{e}^{-(E-E_a)^2/4\omega(x)} P_l(\cos\theta_0)\gamma_l(x'), \tag{4.8}$$

and

$$S_l(x,E) = P_l(\cos\theta_0)S_l(x',E). \tag{4.9}$$

5. Energy deposition for ion transport in multilayer media

We consider a medium consisting of two layers Ω_1 and Ω_2 with thicknesses d_1 and d_2 respectively, where $d_1 \ll d_2$. The ions in second layer Ω_2 have no influence on the transport of the forward-directed ions in the first layer. The ions that scatter back from the second layer to the first, are no longer forward directed and they, if any, would appear in the diffusion ion group. Likewise the forward-directed ions having entered into the second layer Ω_2 would no longer be under the influence of the particles in the first layer. Dealing with the transport of the forward-peaked particles in a certain layer, the layer is virtually extended to a hypersurface with a condition that the fluence of the forward-peaked particles at the boundary is equal to that of the forward-peaked particles in the preceding layer at the same boundary. Considering a multilayer medium is adequate only if there is a difference in the background material in both sides of a layer surface. Such an anisotropy would induce discontinuities in the energy variable. In this study, for simplicity, this discontinuity is assumed to be small and therefore has been neglected. In a medium with a few layers, this assumption introduces a small but negligible approximation error in the model. However, for a medium consisting of a large number of layers, ignoring discontinuities on the inter-layer boundaries would cause accumulative approximation errors that can be an extensive source of inconsistency in the model. To distinguish between the physical quantities of the first layer from those of the second layer, the quantities in the second layer will be denoted by an Astrix $(*)$ on the corresponding quantities from the first layer. Recall that in the first layer Ω_1, we have for $0 \le x \le d_1$, the diffusion ion source is expressed as

$$S_{diff} = \sum_{l=0}^{m} \frac{2l+1}{4\pi} P_l(\mu)S_l(x,E), \qquad S_l = f_{sl}(x,E)\frac{\mathrm{d}}{\mathrm{d}x}\left(\ln\gamma_l(x)\right), \tag{5.1}$$

where f_{sl} is given by (3.32) and

$$\gamma_l(x) = \begin{cases} -\displaystyle\sum_{l'=m+1}^{\infty} D_{ll'}\mathrm{e}^{-C\eta_{l'}q(x)}, & l \le m, \\ 0, & l > m \end{cases} \tag{5.2}$$

with η_l, $D_{ll'}$ and $q(x)$ given by (2.11), (2.15) and (3.34), respectively.

In the second layer the distribution of ions satisfies the following equation and boundary conditions

$$\begin{cases} -\dfrac{\partial(\rho^* f^*)}{\partial E} + \mu^*\dfrac{\partial f^*}{\partial x} - \dfrac{1}{2}\dfrac{\partial^2(\Omega^* f^*)}{\partial E^2} = CE^{-2k}\displaystyle\int_{4\pi} \mathrm{d}\mathbf{u}'[f^*(x,\mu',E) - f^*(x,\mu,E)] \times (1-\mathbf{u}\cdot\mathbf{u}')^{-k-1}, \\ f^*(d_1,\mu,x) = f(d_1,\mu,x), \end{cases} \tag{5.3}$$

on

$$\Omega_2 = \{(x,E) : d_1 \le x \le 1 \,\&\, 0 \le E \le \tilde{E}\},$$

where $\tilde{E} = \min E$; is the minimum amount of the energy deposited on the first layer for $x \in [0, d_1]$. In Ω_2 the distribution function for the forward-directed ions f_s^* and the diffusion ions f_d^* satisfy the following equations:

$$\begin{cases} -\dfrac{\partial(\rho^* f_s^*)}{\partial E} + \mu^*\dfrac{\partial f_s^*}{\partial x} - \dfrac{1}{2}\dfrac{\partial^2(\Omega^* f_s^*)}{\partial E^2} \\ \quad = CE^{-2k}\displaystyle\int_{4\pi} \mathrm{d}\mathbf{u}'[f_s^*(x,\mu',E) - f_s^*(x,\mu,E)] \times (1-\mathbf{u}\cdot\mathbf{u}')^{-k-1} - S_{diff}^*(x,\mu,E), \\ f_s^*(d_1,\mu,E) = f_s(d_1,\mu,E) \end{cases}$$

$$\begin{cases} -\dfrac{\partial(\rho^* f_d^*)}{\partial E} + \mu^* \dfrac{\partial f_d^*}{\partial x} - \dfrac{1}{2}\dfrac{\partial^2(\Omega^* f_d^*)}{\partial E^2} \\ \quad = CE^{-2k} \displaystyle\int_{4\pi} \mathrm{d}\mathbf{u}'[f_d^*(x,\mu',E) - f_d^*(x,\mu,E)] \times (1-\mathbf{u}\cdot\mathbf{u}')^{-k-1} + S_{diff}^*(x,\mu,E), \\ f_d^*(d_1,\mu,E) = f_d(d_1,\mu,E). \end{cases}$$

Performing similar calculations as in previous section, the integral quantities $\gamma_l^*(x)$ of ion transport can be written as

$$\gamma_l^*(x) = \begin{cases} -\displaystyle\sum_{l'=m+1}^{\infty} D_{ll'} \mathrm{e}^{-C\eta_{l'}[q(x)+q^\star(x)]}, & l \le m, \\ 0, & l > m, \end{cases} \tag{5.4}$$

and the spatial component of characteristics are presented by

$$\mu^*(x) = \frac{\int_0^{\tilde{E}} \int_{-1}^{1} \mu f_s^*(x,\mu,E)\mathrm{d}\mu\mathrm{d}E}{\int_0^{\tilde{E}} \int_{-1}^{1} f_s^*(x,\mu,E)\mathrm{d}\mu\mathrm{d}E} = \frac{\int_0^{\tilde{E}} f_{s1}^*(x,E)\mathrm{d}E}{\int_0^{\tilde{E}} f_{s0}^*(x,E)\mathrm{d}E}. \tag{5.5}$$

The equation for f_{sl}^* is then

$$-\frac{\partial}{\partial E}\left[L(E,\Delta) f_{sl}^*(x,E)\right] + \mu_a^*(x)\frac{\partial f_{sl}^*}{\partial x} - \frac{1}{2}\frac{\partial^2}{\partial E^2}\left[\Omega_c^* f_{sl}^*(x,E)\right] = \Gamma_{sl}(f), \tag{5.6}$$

where

$$\Gamma_{sl}(f) := -\begin{cases} \displaystyle\sum_{l'=m+1}^{\infty} CE^{-2k}\eta_{l'} D_{ll'} f_{sl}^*(x,E), & \text{if } l \le m, \\ CE^{-2k}\eta_l f_{sl}(x,E), & \text{if } l > m. \end{cases} \tag{5.7}$$

The very same *approximate* Fourier transformation procedure as before yields

$$\begin{cases} \hat{f}_{sl}^*(x,E) = C^* \mathrm{e}^{-\Lambda^*[x]}, \\ f_{sl}^*(d_1,E) = f_{sl}(d_1,E), \end{cases} \quad C^* = \hat{f}_{sl}(d_1,E)\mathrm{e}^{\Lambda^*[d_1]}. \tag{5.8}$$

Hence

$$\hat{f}_{sl}^*(x,E) = \hat{f}_{sl}(d_1,E)\mathrm{e}^{-\left(\Lambda^*[x]-\Lambda^*[d_1]\right)}. \tag{5.9}$$

Now since

$$\hat{f}_{sl}(d_1,E) = \mathrm{e}^{\Lambda[0]-\Lambda[d_1]-\mathrm{i}\xi E_0} = \mathrm{e}^{-\Lambda[d_1]-\mathrm{i}\xi E_0}, \tag{5.10}$$

thus

$$\hat{f}_{sl}^*(x,E) = \mathrm{e}^{-\left(\Lambda^*[x]-\Lambda^*[d_1]+\Lambda[d_1]\right)} \times \mathrm{e}^{-\mathrm{i}\xi E_0}. \tag{5.11}$$

Consequently

$$f_{sl}^*(x,E) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\xi(E-E_0)} \times \mathrm{e}^{-\left(\Lambda^*[x]-\Lambda^*[d_1]+\Lambda[d_1]\right)}\mathrm{d}\xi. \tag{5.12}$$

Here

$$\Lambda^*[x] = C\eta_l q^*(x) - \mathrm{i}\xi\Delta E_a^*(x) + \xi^2\omega^*(x), \tag{5.13}$$

implies that

$$\Lambda^*[d_1] = C\eta_l q^*(d_1) - \mathrm{i}\xi\Delta E_a^*(d_1) + \xi^2\omega^*(d_1). \tag{5.14}$$

Analogously

$$\Lambda[d_1] = C\eta_l q(d_1) - \mathrm{i}\xi\Delta E_a(d_1) + \xi^2\omega(d_1). \tag{5.15}$$

Thus

$$\begin{aligned} \Lambda^*[x] - \Lambda^*[d_1] + \Lambda[d_1] = {} & C\eta_l\left(q^*(x) - q^*(d_1) + q(d_1)\right) - \mathrm{i}\xi\left(\Delta E_a^*(x) - \Delta E_a^*(d_1) + \Delta E_a(d_1)\right) \\ & + \xi^2\left(\omega^*(x) - \omega^*(d_1) + \omega(d_1)\right). \end{aligned} \tag{5.16}$$

Finally the energy deposition by ions in a two-layer medium is given by the energy integral of zeroth moments of the Legendre coefficients of the straightforward and diffusion fluence functions, (see [33] for the details) viz:

$$D(x) = \begin{cases} \displaystyle\int_0^{E_0} [f_{s0}(x,E) + f_{d0}(x,E)]\,\mathrm{d}E, & 0 \le x \le d_1 \\ \displaystyle\int_0^{\tilde{E}} \left[f_{s0}^*(x,E) + f_{d0}^*(x,E)\right]\mathrm{d}E, & d_1 \le x \le 1. \end{cases} \tag{5.17}$$

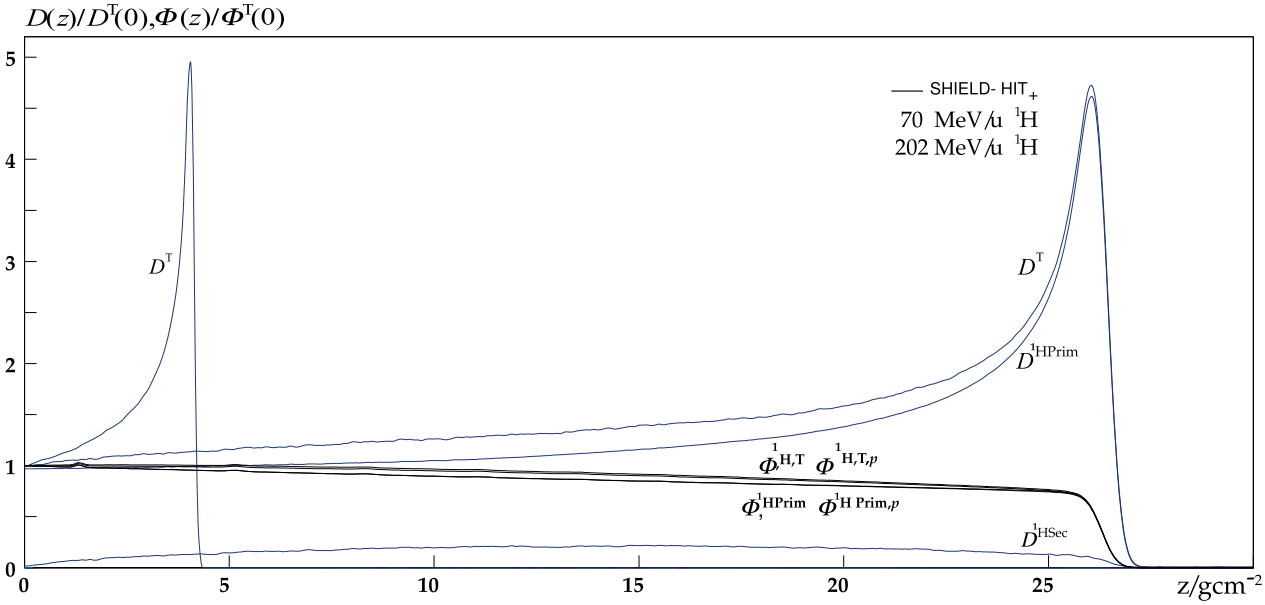

Fig. 3. The total absorbed dose D^T, the primary absorbed dose $D^{1\mathrm{H},T,p}$, the secondary proton dose $\Phi^{H,Sec}$, the total proton fluence $\Phi^{1\mathrm{H},T}$, the total planar proton fluence $\Phi^{1\mathrm{H},T,p}$, the primary fluence $\Phi^{1\mathrm{H},Prim}$, the planar primary fluence $\Phi^{1\mathrm{H},prim,p}$, the secondary protons fluence $\Phi^{1\mathrm{H},\mathrm{Sec}}$, and the planar secondary proton fluence $\Phi^{1\mathrm{H},\mathrm{Sec},p}$ of therapeutic 70 and 202 MeV/u ^{1}H ion beam in water. *SHIELD - HIT + MC* simulations. The curves are normalized to the respective values of the different transport parameters at the phantom surface, $z = 0$.

6. Monte Carlo simulations

The strategy in using Monte Carlo (MC) method, for the bipartition model is governed by taking account the facts characterizing the behavior of the actual problem. During the slowing down of high energy projectiles, fragments are continuously generated, with the origin either from the incoming primary projectile, the target nuclei or by fragments interactions such as those by high energy secondary neutrons, protons, and α-particles. Some of these fragments may therefore be scattered almost isotropically. In the case of a high energy proton beam, the dose from secondary protons is dominating in comparison to other secondaries, cf. [28]. Therefore although, the fact that, in this model we do not consider any absorption term, as given in [30,31], the bipartition model for ion transport, under continuously slowing down assumption, can in the first approximation be related to transport of a therapeutic proton beam. The bipartition model was therefore applied in a case of a therapeutic 70 MeV/u and 202 MeV/u proton beam. In this approach the protons below a specific cutoff angle were treated with the straightforward ion group and thus separated from those protons of more diffusive character. The bipartition model in here is illustrated with the SHIELD-HIT+ MC simulations. The Monte Carlo SHIELD-HIT+ code has advantageous features in implementing radiation for charged particles, see [29,30]. The results are discussed in the aspect of the primary particles fluence, planar fluence and absorbed dose of primary ^{1}H ions and their associated ^{1}H fragments in tissue-like media with ranges of clinical interest.

We calculate the depth absorbed dose distribution of 70 MeV/u and 202 MeV/u ^{1}H ion beams corresponding to ranges of approximately 40 and 260 mm in water. In the present version of, SHIELD-HIT+ code, the fluence differential in both energy and angle was determined both for primary particles and their fragments. The computations are performed for *a point mono-directional and mono-energetic ion beam* perpendicularly incidence at the centre of a cylindrical water phantom (with the radius $R = 10$ cm, and the of length $L = 50$ cm). The fluence or track length per unit volume differential in energy and angle was scored separately in cylindrical rings of a thickness of 1 mm and diameters up to 20 cm. In the plots below the dose represented by $D(z)$ corresponds to $D(x)$ in (5.17) and $\Phi(z)$ to the dept fluence $f(x)$. The plots illustrate protons of forward- and diffusion-directed ion groups for both 70 MeV/u ^{1}H and 202 MeV/u ^{1}H ion beam in water, see [30] for details. Some basic MC codes can be found in [41].

6.1. Summary

We present a mathematical derivation of the bipartition model for low and high energy ion transport in inhomogeneous media with retained energy straggling term: an approach based on an split of the source term to diffusion- and forward-directed particles combined with a Legendre series expansion. We study the problem in single- and multilayer domains as well as obliquely incident case and compute the dose. We employ a modified and new version of simulation code: *SHIELD - HIT+* based on the Monte Carlo method suitable for computations in therapeutic applications.

The results are illustrated in Figs. 3 and 4 that we concisely describe in Fig. 3. the curves have been normalized to the respective values of the different transport parameters at the phantom surface, $z = 0$. In the figures, the total and the

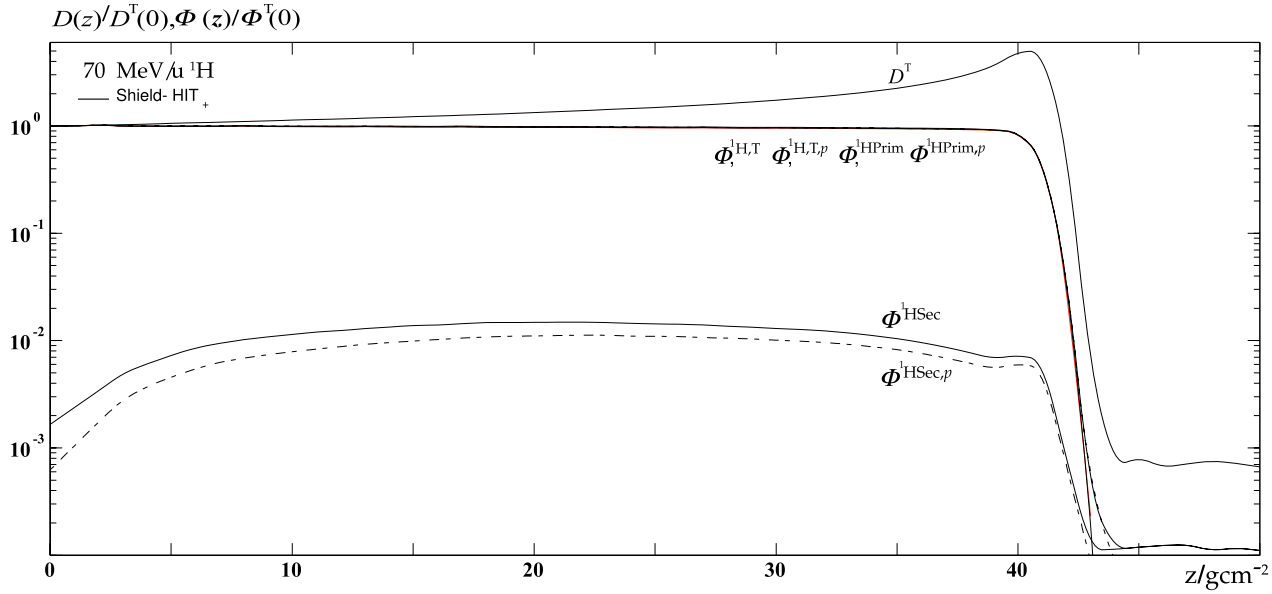

Fig. 4. A close up of the total absorbed dose D^T, the total fluence $\Phi^{1\mathrm{H},T}$, the total planar proton fluence $\Phi^{1\mathrm{H},T,p}$, the primary fluence $\Phi^{1\mathrm{H},prim}$, the planar primary fluence $\Phi^{1\mathrm{H},prim,p}$, the secondary proton fluence $\Phi^{1\mathrm{H},\mathrm{Sec}}$ and the planar secondary protons fluence $\Phi^{1\mathrm{H}\ \mathrm{Sec},p}$ of the therapeutic 70 MeV/u ^{1}H in water. *SHIELD - HIT + MC* simulations. The curves have been normalized to the respective values of the different transport parameters at the phantom surface, $z = 0$.

planar total proton components, are denoted by $\Phi^{1\mathrm{H},T}$ and $\Phi^{1\mathrm{H},T,p}$, respectively. The small differences between these two components illustrate the dominated forward-directed protons. Furthermore from the closed equality between the primary and their associated planar components, i.e. $\Phi^{1\mathrm{H},Prim} \approx \Phi^{1\mathrm{H},Prim,p}$, it is also clear that the diffusion related ion group is closely related to the transport of secondaries Cf. Fig. 4. In Fig. 4 the transport of secondary protons is characterized with the wider angular distribution in contrast to the primary protons as seen by the difference from the planar to the total components. The transport of secondary protons in a high energy proton beam can therefore be associated with the different parts in the discussed bipartition model.

To conclude it is clear that in therapeutic applications, the fluence of forward-directed particles in high energy proton beams, is both related to the transport of primary particles as well as the produced secondary protons. Contributions from the more diffusion scattered protons, are almost solely correlated with the transport of secondary protons and the associated depth dependence of the fluence weighted cosine value, cf. [30]. The bipartition model, with retained energy straggling term, could then be a compliment to other particle transport models to identify the, more isotropically generated and scattered, secondary protons in therapeutic high energy proton beams.

In a forthcoming paper we plan to carry out the analysis for secondary particles and study the bipartition and discontinuous Galerkin finite element methods for this setting.

Acknowledgements

We are grateful to Dr Gou Chengjun for all discussions and his invaluable comments.

The research of the first author is supported by the Swedish Foundation of Strategic Research (SSF) in Gothenburg Mathematical Modeling Centre (GMMC).

References

[1] E.W. Larsen, Liang Liang, The atomic mix approximation for charged particle transport, SIAM, J. Appl. Math. 68 (2007) 43–58.
[2] G.C. Pomraning, The Fokker–Planck operator as an asymptotic limit, Math. Models Methods Appl. Sci. 2 (1992) 21–36.
[3] G.C. Pomraning, The transport theory of beams, Transport Theorey Statist. Phys. 29 (2000) 1–41.
[4] E.W. Larsen, The nature of transport calculations in radiation oncology, Transport Theorey Statist. Phys. 26 (1997) 739.
[5] E.W. Larsen, Asymptotic derivation of the atomic-mix diffusion model for 1-D random media, Trans. Am. Nucl. Soc. 89 (2003) 296–297.
[6] M. Asadzadeh, A. Brahme, J. Xin, Galerkin methods for primary ion transport in inhomogeneous media, Kinet. Relat. Models 3 (2010) 373–394.
[7] M. Asadzadeh, On the stability of characteristic schemes for the Fermi equation, Appl. Comput. Math. 1 (2002) 158–174.
[8] M. Asadzadeh, The Fokker–Planck operator as an asymptotic limit in anisotropic media, Math. Comput. Modelling 35 (2002) 1119–1133.
[9] M. Asadzadeh, A posteriori error estimates for the Fokker–Planck and Fermi pencil beam equations, Math. Models Methods Appl. Sci. 10 (2000) 737–769.
[10] M. Asadzadeh, Streamline diffusion methods for the Fermi and Fokker–Planck Equations, Transport Theory Statist. Phys. (1997) 319–340.
[11] N. Bellomo, P. Maini, Preface(special issue on cancer modelling), Math. Models Methods Appl. Sci. 15 (Suppli., iii–viii) (2005).
[12] N. Bellomo, P. Maini, Preface(special issue on cancer modelling), Math. Models Methods Appl. Sci. 16 (Suppli., iii–vii) (2006).
[13] N. Bellomo, P. Maini, Preface–Challenging mathematical problems in cancer modelling, Math. Models Methods Appl. Sci. 17 (Suppl.) (2007) 1641–1645.
[14] N. Bellomo, N.K. Li, P. Maini, On the foundations of cancer modelling: Selected topics, speculations, and perspectives, Math. Models Methods Appl. Sci. 18 (4) (2008) 593–646.

[15] M. Frank, M. Herty, M. Schäfer, Optimal treatment planning in radiotherapy based on Boltzmann transport calculations, Math. Models Methods Appl. Sci. 18 (2008) 573–592.
[16] M. Frank, M. Herty, A. Sandjo, Optimal radiotherapy treatment planning governed by kinetic equations, Math. Models Methods Appl. Sci. 20 (2010) 661–678.
[17] Baochang Shi, Bin Deng, Rui Du, Xingwang Chen, A new scheme for source term in LBGK model for convection–diffusion equation, Comput. Math. Appl. (2008) 1560–1567.
[18] Maik Stiebler, Jonas Tölke, Manfred Krafczyk, Advection–diffusion lattice Boltzmann scheme for hierarchical grids, Comput. Math. Appl. (2008) 1576–1584.
[19] C. Bianca, F. Pappalardo, S. Motta, The MVF method for kinetic equations system, Comput. Math. Appl. 57 (2009) 831–840.
[20] Pietro Asinari, Taku Ohwada, Connection between kinetic methods for fluid-dynamic equations and macroscopic finite-difference schemes, Comput. Math. Appl. (2009) 841–861.
[21] E.E. Lewis, W.F. Miller Jr., Computational Methods of Neutron Transport, John Wiley & Sons, New York, 1984.
[22] Z. Luo, S. Wang, Bipartition model of ion transport: an outline of new range theory for light ions, Phys. Rev. B 36 (1987) 1885–1893.
[23] J. Coderre, Lecture notes in Principles of Radiation interactions, Department of Nuclear science and Engineering, MIT, Fall, 2004.
[24] D. Belkic, K. Belkic, Decisive role of mathematical methods in early cancer diagnostics: optimized Pade-based magnetic resonance spectroscopy, J. Math. Chem. 42 (2007) 1–35.
[25] I. Lax, A. Brahme, Electron beam dose planing using Gaussian beams: energy and spatial scaling with inhomogeneities, Acta Radiol. Oncol. 24 (1985) 75–85.
[26] A. Brahme, I. Lax, Dose distribution of electron beams in uniform and inhomogeneous media, Acta Radiol. 364 (Suppl.) (1983) 61–72.
[27] A. Brahme, J. Nilsson, D. Belkic, Biologically optimized radiation therapy, Acta Oncologica 40 (2001) 725–734.
[28] J. Kempe, I. Gudowska, A. Brahme, Depth absorbed dose and LET distributions of therapeutic H, He^4, Li^7 and C12, Med. Phys. 34 (2007) 183–192.
[29] J. Kempe, A. Brahme, Energy-range relation and mean energy variation in therapeutic particle beams, Med. Phys. 35 (2008) 159–170.
[30] J. Kempe, A. Brahme, Analytical theory for the fluence, planar fluence, energy fluence, planar energy fluence and absorbed dose of primary particles and their transport in light ion beams, Phys. Med. 26 (2010) 6–16.
[31] J. Kempe, A. Brahme, Solution of the Boltzmann equation for primary light ions and their fragments, preprint, Division of Medical Radiation Physics, Department of Oncology-Pathology, Karolinska Institute and Stockholm University.
[32] Z. Luo, Improved bipartition model for electron transport. I. A general formulation, Phys. Rev. B 32 (1985) 812–823.
[33] Z. Luo, Improved bipartition model for electron transport. II. Application to inhomogeneous media, Phys. Rev. B 32 (1985) 824–836.
[34] Z. Luo, C. Gou, W. Laub, The penetration, diffusion and energy deposition of high-energy photon, reprint, Inst of Nuclear Science and Technology, Sichuan University, China and Radiation Oncology, William Beaumont Hospital, Michigan, USA, 2000.
[35] J. Nilsson, B. Lind, A. Brahme, Radiation response of hypoxic and generally heterogeneous tissues, Int. J. Radiat. Biol. 78 (2002) 389–405.
[36] V.I. Arnold, in: Richard A. Silverman. (Ed.), Ordinary Differential Equations, 2nd ed., MIT Press, Cambridge, Massachusetts, and London, England, 1980.
[37] G.B. Folland, Fourier Analysis and its Applications, Brooks/Cole Publishing Company, A division of International Thomson Publishing Company, USA, 1992.
[38] J.C. Mark, Natural Resource Council of Canada, Report No MT-92, 1944 (unpublished); MT-97, 1945 (unpublished).
[39] R.E. Marshak, Note on the spherical harmonic method as applied to the Milne problem for a sphere, Phys. Rev. (2) 71 (1947) 443–446.
[40] Samuel S. Holland Jr., Applied Analysis by the Hilbert Space Method, Marcel Dekker Inc., New York and Basel, 1990.
[41] J.A. Antolak, M.S. Bieda, K.R. Hogstrom, Monte Carlo Method for commissioning electron beams, in: W. Schlegel, T. Bortfeld (Eds.), The Use of Computers in Radiation Therapy, Springer-Verlag, Berlin, 2000, pp. 449–451.
[42] Z. Luo, A. Brahme, High energy electron transport, Phys. Rev. B 46 (1992) 739–752.