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1

ION TRANSPORT IN INHOMOGENEOUS MEDIA I. BIPARTITION MODEL FOR PRIMARY IONS

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Dedicated to the memory of Luo Zheng-Ming

ABSTRACT. The present paper concerns a mathematical modeling procedure for the charged particle transport and is part I of an investigation organized in two parts. We study the energy deposition of high-energy ($\approx 50-500$ MeV) protons (high-energy electrons in energy range up to 50 MeV) in inhomogeneous media. This work is an extension of the bipartition model for high-energy electrons studied by Luo and Brahme in [27], and light ions studied by Luo and Wang in [29], to *high-energy* ions in inhomogeneous media with 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. 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 type 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 analytic broad beam model of the light- and high-energy ion absorbed dose were compared with the results of a modified Monte Carlo code: SHIELD-HIT. Part II concerns stability and convergence analysis for the semi-discrete, fully discrete, and the streamline diffusion, Galerkin approximations of a such obtained convection-diffusion equation for the broad beam model and is the subject of a forthcoming paper.

1. INTRODUCTION

Charged particles entering into a medium undergo multiple elastic and inelastic collisions. The elastic collisions that result are alternating 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-directness assumption, only a very small portion of the ions is scattered to *large angles*. These are, except at very low energies, very few ions with a directional change beyond a certain minimal angle θ_m, determined by the *bipartition condition below*, which have a *diffusion-like* transport behavior and an, almost, isotropic angular distribution. Hence, their

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transport behavior is, preferably, described using P_n -approximations of spherical harmonics. The remaining significant portion of the ion particles, deflecting slightly ($< \theta_m$) from the original direction, are convective ions and refereed to as *forward-directed* ions. Their transport behavior is described in terms of the small-angle approximations. To separate the large-angle scattered and forward-directed ions properly, the partition condition is introduced. The current model is based on a split, of the scattering integral (kernel), through adding and 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 [20]. This kind of splitting strategy is more common in medical physics studies related to the application of radiation particle beams (see Section 6) in cancer therapy.

We perform this study in a mathematical modeling and a numerical approximation part: In the modeling procedure the underlying physics is for the case of ions injected into a background medium with large atomic weight. Here, we have considered transport phenomena 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, see [36]. The second part is the subject of a forthcoming paper, where we deal with the finite element approximations for the convection diffusion equation in part I, corresponding to asymptotically derived broad beam equation. For the asymptotic expansion procedure and some studies of resulting pencil beam equations see, e.g. [36]-[37], [17]-[20] and [2]-[5].

In the present paper, we study an ion transport model describing the actual process of energetic ions in absorbing media. To this end we let $f(\mathbf{x}, \mathbf{v}, E)$ denote the ion distribution function which is also called the *ion fluence differential* in angle and energy. Then $f(\mathbf{x}, \mathbf{v}, E)d\mathbf{v}dE$ represents the ion fluence at point $\mathbf{x} \in \mathbb{R}^3$, with direction between $\mathbf{v}$ and $\mathbf{v}+d\mathbf{v}$ and energy between E and $E+dE$ ($\mathbf{v} \in \mathbb{R}^3$, $E \in \mathbb{R}^+$). 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]

$$\begin{aligned} \mathbf{v} \cdot \nabla_{\mathbf{x}} f - \frac{\partial(\rho f)}{\partial E} &= \frac{1}{2}\frac{\partial^2(\Omega f)}{\partial E^2} + N \int_{4\pi} d\mathbf{v}' \{[f(\mathbf{x}, \mathbf{v}', E) - f(\mathbf{x}, \mathbf{v}, E)] \times \\ &\quad \times \sigma_n(E', 2E(1 - \mathbf{v} \cdot \mathbf{v}')M_1/M_2)\} + S(\mathbf{x}, \mathbf{v}, E), \end{aligned} \tag{1.1}$$

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 $M_1 << M_2$) and S is the ion source term. Although we do not assume light ion particles where in each collision an ion can transfer only a small fraction of its energy to the medium, nevertheless we assume a continuous slowing down approximation (CSDA) to justify for the collision integral formulated as above in (1.1) as well as the presence of the *energy-loss straggling* term $-\frac{1}{2}\frac{\partial^2(\Omega f)}{\partial E^2}$. In the study for light ion transport, see [29], 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 [29] and the references therein, for proton, helium and carbon ions, we have assigned an inverse polynomial approximation for the cross-section term in form of separated inverse *power functions* in E and $1-\mathbf{v}\cdot\mathbf{v}'$. Different forms of power approximation are considered in the particle transport. For some relevant forms in radiation interactions see, e.g. [9].

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. [7]- [8], [13]- [16], [22]-[30] and [35].

The outline of this paper is as follows: In section 2 we start with the ion transport equation under the *Continuous Slowing Down Assumption* (CSDA) and derive a computable form of the partition condition and bipartition coefficients. We skip discussions on the relevant range of elastic, inelastic and bremsstrahlung cross-sections for this derivation. Such physical discussions can be found in [22]-[30] and the references therein. 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 straight forward particles, as well as the Legendre coefficients S_l for the diffusion source. Due to the algebraic fall-off assumption for the kernel, both parameters are derived by approximation in an inverse 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 method.

2. Bipartition model for ion transport under CSDA

To describe the transport of ions of, e.g., 50 MeV to $\approx$ 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, where both left and right side of the hyper-surface are assumed to be composed of the same medium. (In Section 5 we shall include the case when the left half-space is vacuum). 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 ion transport equation under the CSDA is given by

$$\begin{aligned}(2.1)\qquad -\frac{\partial(\rho f)}{\partial E}+\mu\frac{\partial f}{\partial x}-\frac{1}{2}\frac{\partial^2(\Omega f)}{\partial E^2} &:= \tilde{\delta}+C_f\equiv\frac{1}{2\pi}\delta(x)\delta(E-E_0)\delta(1-\mu)\\ &+CE^{-2k}\int_{4\pi}d\mathbf{v}'[f(x,\mu',E)-f(x,\mu,E)]\times(1-\mathbf{v}\cdot\mathbf{v}')^{-k-1},\end{aligned}$$

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 $\mathbf{v}$, passing through a unit distance, caused by elastic scattering.

From the equation (2.2) and the property that the small-angle elastic scattering of ions is dominating, the main characteristics of C_f can be featured as shown in Fig 1. below.

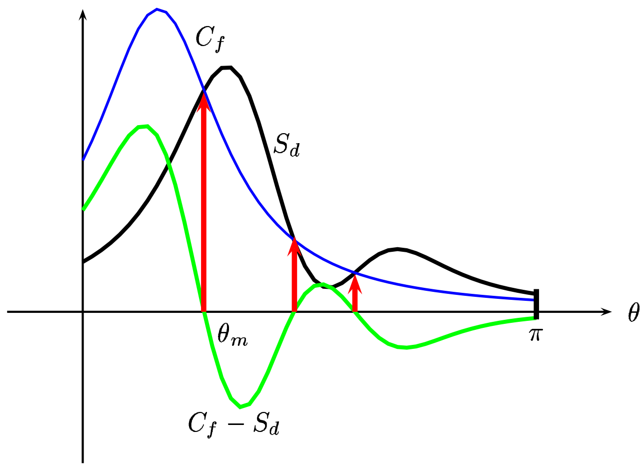

Figure 1: The extract of diffusion source S_d from the collision term C_f.

In the bipartition strategy for particle transport, 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. The latter, convective part, is normally of negative value, indicating that the number of ions that leave the forward small-angle direction due to elastic scattering is larger than that of ions that enter the small-angle directions caused by elastic scattering. For our physical model we have considered a scattering kernel with strong algebraic fall-off behavior from its peaks at zero angle and zero energy. To this end we have assumed an inverse power function approximation for the elastic cross-section for ion transport, (see also [9]), viz

$$\sigma_n(E, \mathbf{v}\cdot\mathbf{v}') \approx CE^{-2k}(1-\mathbf{v}\cdot\mathbf{v}')^{-1-k}, \tag{2.2}$$

where C is a constant depending on E_0, atomic numbers and also Bohr radius (a factor of the classical electron radius, see [29] for details), k is a positive integer which corresponds to the magnitude of the algebraic fall-offs.

To solve for spherical harmonic coefficients by using Fourier transformation, (2.2) would enforce yet another approximation in computing Fourier integrals. Singular terms of the form (2.2) are not treated/appeared in a general (non-approximative) splitting strategy. 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

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

and f_d is the distribution of the diffusion ion particles satisfying

$$\begin{aligned}(2.5)\qquad -\frac{\partial(\rho f_d)}{\partial E} + \mu\frac{\partial f_d}{\partial x} - \frac{1}{2}\frac{\partial^2(\Omega f_d)}{\partial E^2} &= s_d +\\ &+ CE^{-2k}\int_{4\pi} d\mathbf{v}'[f_d(\mathbf{x},\mu',E) - f_d(x,\mu,E)] \times (1-\mathbf{v}\cdot\mathbf{v}')^{-k-1}.\end{aligned}$$

Physically, the collision term represents a scattering source. Thus, using the bipartition model we deduct the large-angle scattering source from the collision term in the straight-forward ion transport equation (2.1) 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 ion transport equation (2.1). *The partition condition* is given by

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

The condition (2.6) shows that all the large-angle scattered ions in the straight-forward 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,

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

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

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

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

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

where

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

Obviously $\eta_0 = 0$ and for $l \geq 1$, η_l can be obtained by the following recursive formula:

Lemma 2.1. *([29]) The collision coefficient η_l satisfies the recurrent relation*

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

Proof. Recall the following recurrent formulas for the Legendre polynomials:

$$(l+1)P_{l+1}(\mu) = \mu P'_{l+1}(\mu) - P'_l(\mu), \tag{2.13}$$

$$(l+1)P_l(\mu) = P'_{l+1}(\mu) - \mu P'_l(\mu). \tag{2.14}$$

Subtraction (2.13) from (2.14) we obtain

$$(l+1)[P_l(\mu) - P_{l+1}(\mu)] = (1-\mu)[P'_{l+1}(\mu) + P'_l(\mu)]. \tag{2.15}$$

Thus, we can use partial integration resulting in:

$$(l+1)\int_{-1}^{1}[P_l(\mu) - P_{l+1}(\mu)](1-\mu)^{-1-k}\,d\mu = [P_{l+1}(\mu) + P_l(\mu)](1-\mu)^{-k}\Big|_{-1}^{1}$$
$$- k\int_{-1}^{1}[P_{l+1}(\mu) + P_l(\mu)](1-\mu)^{-1-k}\,d\mu.$$

Since, $\forall n,\ P_n(-x) = (-1)^n P_n(x)$ and $P_n(1) = 1$, the contribution from the boundary term vanishes and we end up with

$$(l+1+k)\int_{-1}^{1}P_l(\mu)(1-\mu)^{-1-k}\,d\mu = (l+1-k)\int_{-1}^{1}P_{l+1}(\mu)(1-\mu)^{-1-k}\,d\mu, \tag{2.16}$$

which, to extract η_l and η_{l+1}, can be rewritten as

$$(l+1-k)\int_{-1}^{1}[1 - P_{l+1}(\mu)](1-\mu)^{-1-k}\,d\mu - (l+1-k)\int_{-1}^{1}(1-\mu)^{-1-k}\,d\mu$$
$$= (l+1+k)\int_{-1}^{1}[1 - P_l(\mu)](1-\mu)^{-1-k}\,d\mu - (l+1+k)\int_{-1}^{1}(1-\mu)^{-1-k}\,d\mu.$$

i.e.,

$$(l+1-k)\eta_{l+1}/2\pi - (l+1+k)\eta_l/2\pi = -2k\int_{-1}^{1}(1-\mu)^{-1-k}\,d\mu = 2^{1-k}, \tag{2.17}$$

and we have the desired recurrent formula as stated in the lemma. □

Note that inserting (2.10) into (2.6) and using (2.9) we get a more specific partition condition viz,

$$-CE^{-2k}\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}\eta_l P_l(\mu_i) f_{sl}(x,E) = \sum_{l=0}^{m}\frac{2l+1}{4\pi}P_l(\mu_i) S_{dl}(x,E). \tag{2.18}$$

Therefore

$$S_{dl}(x,E) = -CE^{-2k}\Big(\eta_l f_{sl}(x,E) + \sum_{l'=k+1}^{\infty}\eta'_l D_{ll'} f_{sl'}(x,E)\Big). \tag{2.19}$$

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

$$D_{ll'} = \frac{2l'+1}{2l+1}\cdot\frac{\Delta_{ll'}}{\Delta_l}, \tag{2.20}$$

where we 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

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

Further discussions on *the small-angle condition* and other quantities can be found in [22]-[30].

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: $C_f(x,\mu_i,E) = S_d(x,\mu_i,E),\ i=0,1,\dots,m$,

(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 so called small-angle approximation is to substitute μ in the term $\mu(\partial f_s/\partial x)$ by $\mu_a(x)$ an average direction cosine given by

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

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 as above and consequently, to transfer the equation for f_s to an ordinary differential equation (ODE), 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

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

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

where $L(E,E')$ is an approximation of the conventional stopping power ρ. In this way we end up with the equation for the Legendre coefficients f_{sl} as

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

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

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

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

Following [27], one can show that

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

Therefore, as soon as, we obtain a solution of (3.5), we automatically have a solution for (3.4) as well. To obtain a solution for (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}, $(k>0)$. Therefore 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;

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

where

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

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

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

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

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

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

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), $\int_{-\infty}^{\infty} g(x,E)\, dE \approx 1$, i.e. $g \in L_1$. Taking Fourier transform of (3.11) we get

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

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 $g(x,E) \approx \delta_x(E)$, see Folland [10], chapter 7, we may chose an approximation of the form:

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

The goal, in this procedure, is to give a closed form solution for $\hat{f}_{sl}$, then by the inverse Fourier transform we can get the l-th Legendre components f_{sl}. To this approach it suffices to invoke, in the *forward peakedness* assumption, 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., recalling (3.11), we approximate $g := w/w_a$ by the Dirac δ function in energy variable. Hence

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

This however is *too general*: in reality our energy variable ranges in an interval $I = [0_-, E_0]$ (0_-, to avoid integrating $\delta(E)$ over I) and a more suitable approach would be just using the *integral form of the generalized mean value theorem* :

Lemma 3.3 (generalized mean value theorem for integrals). *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*

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

Hence the indefinite integral in (3.7) can be replaced by a definite 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 these simple and somewhat physically motivated manipulations, the Fourier transform of (3.5), with respect to E yields the approximate equation

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

i.e.,

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

To simplify we write this relation as

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

or equivalently

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

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

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

i.e.,

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

We introduce the substitution $x \to y$ and integrate over $(0,x)$ to obtain

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

Recall that $\mu(x)$ is the cosine of the angle between the direction of the ions and the x-axis. Thus starting with the straight-forward ions $\mu_a(0) \approx 1$, and consequently we may write

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

Note that

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

Obviously, this identification yields $q(0) = \Delta E(0) = \omega(0) = 0$, and consequently $\Lambda(0) = 0$. Further, assuming vacuum condition to the left of $x = 0$ we get

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

Hence

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

Thus we have

$$\begin{aligned} f_{sl}(x,\xi) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{1}{\mu_a(0)} e^{i\xi E} \cdot e^{-i\xi(E_0-\Delta E(x)) - C\eta_l q(x) - \xi^2\omega(x)}\,d\xi \\ &= \frac{1}{2\pi} e^{-C\eta_l q(x)} \int_{-\infty}^{\infty} e^{i\xi E} \cdot e^{-i\xi(E_0-\Delta E(x))} \cdot e^{-\xi^2\omega(x)}\,d\xi. \end{aligned} \tag{3.25}$$

We define

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

Comparing with the inverse Fourier transform

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

we have that

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

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

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

Then, with $E_a = E_0 - \Delta E$ we may write

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

so that finally we get

$$\begin{aligned} f_{sl}(x,E) &= \frac{1}{2\pi}\sqrt{\frac{\pi}{\omega(x)}} e^{-[E-(E_0-\Delta E)]^2/4\omega(x)} \cdot e^{-C\eta_l q(x)} \\ &= \frac{1}{2\pi}\sqrt{\frac{\pi}{\omega(x)}} e^{-(E-E_a)^2/4\omega(x)} \cdot e^{-C\eta_l q(x)}. \end{aligned} \tag{3.31}$$

Thus, recalling (3.4) and (3.5)the Legendre coefficients of the distribution function f can be written as

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

where

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

At this point, as in the case of equations (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, recall that

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

Having computed f_{sl}, then we can give a more, numerically, computable formula for $S_l(x,E)$ than the formal derivation of the form (2.20) and prepare for the study of the diffusion ion group.

Proposition 3.4. *For the bipartition model the Legendre coefficients $S_l(x,E)$ for the diffusion source term in* (2.20) *are given by*

$$S_l(x,E)=\Big[-CE^{-2k}\eta_l+\frac{d}{dx}\ln\Big(\gamma_l(x)\Big)\Big]f_{sl}(x,E). \tag{3.35}$$

Proof. Differentiating (3.32) we have

$$\frac{\partial f_{sl}}{\partial E}=\Big[-\frac{E-E_a}{2\omega}\Big]f_{sl}. \tag{3.36}$$

Using (3.36) we get

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

Further

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

where, to get 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 using the auxiliary relations

$$\frac{d\omega}{dx}=\frac{\Omega_c}{2\mu_a},\quad \frac{dE_a}{dx}=\frac{l}{\mu_a}, \tag{3.38}$$

we immediately get

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

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

$$(3.40)\qquad S_l(x,E)=\Big[-CE^{-2k}\eta_l+\frac{d}{dx}\ln\Big(\gamma_l(x)\Big)\Big]f_{sl}(x,E),$$

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

3.2. **The diffusion ion group.** With the diffusion coefficients S_l 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 cut-off method, based on P_n-approximation, is commonly used assuming

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

and hence, a weighted central differencing, see [29] and [23] for details, yields

$$(3.42)\qquad \begin{aligned} -\frac{\partial(\rho f_{dl})}{\partial E}+\frac{1}{2l+1}\Big[(l+1)\frac{\partial(\mu_a f_{d,l+1})}{\partial x}+l\frac{\partial(\mu_a f_{d,l-1})}{\partial x}\Big]-\frac{1}{2}\frac{\partial^2(\Omega f_{dl})}{\partial E^2}\\ =-CE^{-2k}\eta_l f_{dl}+\tilde S_l(x,E),\qquad l=0,1,\dots,n,\end{aligned}$$

where

$$(3.43)\qquad \tilde S_l(x,E):=f_{sl}(x,E)\frac{d}{dx}\ln\Big(\gamma_l(x)\Big),\qquad l=0,1,\dots,n.$$

Under certain assumptions on the coefficients, this set of equations may have closed form analytic solutions. But, in the real application problems, the coefficients are often rather involved expressions and therefore numerical methods are the most realistic and desirable approaches. For a reliable numerical method the stability of the discrete scheme is essential. A direct approach is based on a Lax-Wendroff scheme applied to a symmetrical form of (3.42) for the auxiliary function $\tilde f_{dl}$, below

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

The function $\tilde f_{dl}$ would satisfy the following, second order accurate, scheme:

$$(3.45)\qquad \begin{aligned} -\frac{\partial(\rho\tilde f_{dl})}{\partial E}=-\frac{1}{\sqrt{2l+1}}\Big[\frac{l+1}{\sqrt{2l+3}}\frac{\partial(\mu_a\tilde f_{d,l+1})}{\partial x}+\frac{l}{\sqrt{2l-1}}\frac{\partial(\mu_a\tilde f_{d,l-1})}{\partial x}\Big]\\ -\frac{1}{2}\frac{\partial^2(\Omega\tilde f_{dl})}{\partial E^2}-CE^{-2k}\eta_l\tilde f_{dl}+\frac{1}{\sqrt{2l+1}}\tilde S_l,\qquad l=0,1,\dots,n.\end{aligned}$$

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

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

The equation (3.45) is a degenerate type convection-diffusion equation which is studied extensively in [2]-[5] using, e.g. the *Streamline diffusion* finite element method. In our standard Galerkin study in Section 6 we consider a general form of

(3.46) with somewhat more specified coefficients. In a forthcoming paper we shall study a discontinuous Galerkin method for approximating the solution for (3.46).

3.3. **Boundary conditions.** For the semi infinite media we account for the condition for the bipartition theory being applied to semi-infinite surface of solid. As the left half-space is vacuum, expecting the incident ions, only the ions reflected from the solid surface to the left-hand side vacuum may exist at the boundary $x = 0$. Therefore it is reasonable to assume, a boundary condition of the form,

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

This is the vacuum boundary condition. 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 [31], Marshak [32] and Marshak. Both conditions are assuming an odd number of discrete cosine directions; n. The Mark condition is based on treating the left-hand-side vacuum as a scape black-box in the sense that: the ions leaving the solid surface no longer return to the solid. This condition reads as follows:

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

The Marshak condition is formulated for the current; ensuring that no diffusion ion current is incident upon the solid surface from the vacuum, and thus reads as follows:

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

Mark condition is used for higher degree approximations 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 equation (3.46) additional conditions are supplied for $\mu < 0$. These are of the form

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

and are described more closely in [29] and the references therein. Now with the complete number of boundary conditions the model is ready to expand to the study of the multilayer case of ion transport.

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 the Fig.1 below: 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 ion particles. To proceed

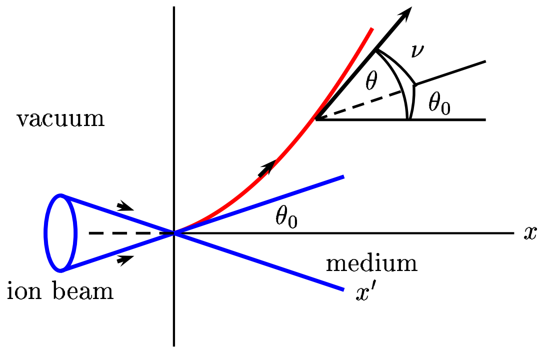

Figure 2: Obliquely incident ions.

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

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

and

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

Now we may return to the original coordinate system, recalling

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

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

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

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

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

Thus

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

Using the addition theorem of Legendre polynomials, we have

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

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 $d_1 << d_2$. 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 diffuse 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 the 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. In a forthcoming study, using a discontinuous Galerkin finite element method, we tackle problems with a pronounced discontinuity in the energy variable. For the sake of comparison we also study the convergence of the standard Galerkin finite element method for the convection diffusion problem corresponding to the present model (with neglected discontinuities). 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 $0 \le x \le d_1$ and

$$
f_s(x,\mu,E) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} P_l(\mu) f_{sl}(x,E), \tag{5.1}
$$

$$
f_{sl}(x,E) = \frac{1}{2\pi}\sqrt{\frac{\pi}{\omega(x)}} e^{-(E-E_a)^2/4\omega(x)} \gamma_l(x) \tag{5.2}
$$

where

$$\omega(x) = \frac{1}{2}\int_0^x \frac{\Omega_c[E_a(x')]}{\mu_a(x')}\,dx', \quad \text{with} \quad \mu_a(x) = \frac{\int_0^{E_0} f_{s1}(x,E)\,dE}{\int_0^{E_0} f_{s0}(x,E)\,dE}, \tag{5.3}$$

$$E_a(x) = E_0 - \int_0^{L_a} L(E,E')\,dL', \qquad L_a = \int_0^x \frac{1}{\mu_a(x')}\,dx', \tag{5.4}$$

and

$$\gamma_l(x) = \begin{cases} -\sum_{l'=m+1}^{\infty} D_{ll'} e^{-C\eta_{l'} q(x)}, & l \le m, \\ 0, & l > m. \end{cases} \tag{5.5}$$

with

$$\eta_l = 2\pi \int_{-1}^{1} [1 - P_l(\mu)](1-\mu)^{-k-1}\,d\mu \quad \text{and} \quad q(x) = \int_0^x \frac{E_a(x')^{-2k}}{\mu_a(x')}\,dx'. \tag{5.6}$$

Further the diffusion ion source is expressed as

$$S_{diff} = \sum_{l=0}^{m} \frac{2l+1}{4\pi} P_l(\mu) S_l(x,E), \qquad S_l = f_{sl}(x,E)\frac{d}{dx}\Big(\ln \gamma_l(x)\Big). \tag{5.7}$$

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

$$\begin{cases} -\dfrac{\partial(\rho^* f^*)}{\partial E} & +\mu^*\dfrac{\partial f^*}{\partial x} - \dfrac{1}{2}\dfrac{\partial^2(\Omega^* f^*)}{\partial E^2} = CE^{-2k}\times \\ & \displaystyle\int_{4\pi} d\mathbf{v}'[f^*(\mathbf{x},\mu',E) - f^*(x,\mu,E)] \times (1 - \mathbf{v}\cdot\mathbf{v}')^{-k-1}, \\ f^*(d_1,\mu,x) & = f(d_1,\mu,x), \end{cases} \tag{5.8}$$

on

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

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:

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

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

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

$$\gamma_l^*(x) = \begin{cases} -\sum_{l'=m+1}^{\infty} D_{ll'} e^{-C\eta_{l'}[q(x)+q^*(x)]}, & l \le m, \\ 0, & l > m. \end{cases} \tag{5.9}$$

$$\mu^*(x) = \frac{\int_0^{\tilde{E}} \int_{-1}^{1} \mu f_s^*(x,\mu,E)\, d\mu\, dE}{\int_0^{\tilde{E}} \int_{-1}^{1} f_s^*(x,\mu,E)\, d\mu\, dE} = \frac{\int_0^{\tilde{E}} f_{s1}^*(x,E)\, dE}{\int_0^{\tilde{E}} f_{s0}^*(x,E)\, dE}. \tag{5.10}$$

The equation for f_{sl}^* is then

$$-\frac{\partial}{\partial E}\Big[L(E,\Delta) f_{sl}^*(x,E)\Big] + \mu_a^*(x)\frac{\partial f_{sl}^*}{\partial x} - \frac{1}{2}\frac{\partial^2}{\partial E^2}\Big[\Omega_c^* f_{sl}^*(x,E)\Big] = \Gamma_{sl}(f), \tag{5.11}$$

where

$$\Gamma_{sl}(f) := -\begin{cases} \sum_{l'=m+1}^{\infty} CE^{-2k}\eta_{l'} D_{ll'} f_{sl}^*(x,E), & \text{if } l \le m, \\ CE^{-2k}\eta_l f_{sl}(x,E), & \text{if } l > m. \end{cases} \tag{5.12}$$

The very same *approximative* Fourier transformation procedure as before (bearing in mind that some of the equalities below are derived with negligible approximation errors) yields

$$\begin{cases} \hat{f}_{sl}^*(x,E) = C^* e^{-\Lambda^*[x]}, \\ f_{sl}^*(d_1,E) = f_{sl}(d_1,E), \end{cases} \qquad C^* = \hat{f}_{sl}(d_1,E) e^{\Lambda^*[d_1]}. \tag{5.13}$$

Hence

$$\hat{f}_{sl}^*(x,E) = \hat{f}_{sl}(d_1,E) e^{-\left(\Lambda^*[x]-\Lambda^*[d_1]\right)}. \tag{5.14}$$

Now since

$$\hat{f}_{sl}(d_1,E) = e^{\Lambda[0]-\Lambda[d_1]-i\xi E_0} = e^{-\Lambda[d_1]-i\xi E_0}, \tag{5.15}$$

thus

$$\hat{f}_{sl}^*(x,E) = e^{-\left(\Lambda^*[x]-\Lambda^*[d_1]+\Lambda[d_1]\right)} \times e^{-i\xi E_0}. \tag{5.16}$$

Consequently

$$f_{sl}^*(x,E) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\xi(E-E_0)} \times e^{-\left(\Lambda^*[x]-\Lambda^*[d_1]+\Lambda[d_1]\right)}\, d\xi. \tag{5.17}$$

Here

$$\Lambda^*[x] = C\eta_l q^*(x) - i\xi\Delta E_a^*(x) + \xi^2\omega^*(x), \tag{5.18}$$

implies that

$$\Lambda^*[d_1] = C\eta_l q^*(d_1) - i\xi\Delta E_a^*(d_1) + \xi^2\omega^*(d_1). \tag{5.19}$$

Analogously

$$\Lambda[d_1] = C\eta_l q(d_1) - i\xi\Delta E_a(d_1) + \xi^2\omega(d_1). \tag{5.20}$$

Thus

$$\begin{aligned} \Lambda^*[x] - \Lambda^*[d_1] + \Lambda[d_1] = {} & C\eta_l\Big(q^*(x) - q^*(d_1) + q(d_1)\Big) \\ & - i\xi\Big(\Delta E_a^*(x) - \Delta E_a^*(d_1) + \Delta E_a(d_1)\Big) \\ & + \xi^2\Big(\omega^*(x) - \omega^*(d_1) + \omega(d_1)\Big). \end{aligned} \tag{5.21}$$

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 straight-forward and diffusion fluence functions, (see [23] for the details) viz:

$$D(x) = \begin{cases} \displaystyle\int_0^{E_0} \Big[f_{s0}(x,E) + f_{d0}(x,E)\Big]\, dE, & 0 \le x \le d_1 \\ \displaystyle\int_0^{\tilde{E}} \Big[f^*_{s0}(x,E) + f^*_{d0}(x,E)\Big]\, dE, & d_1 \le x \le 1. \end{cases} \tag{5.22}$$

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 by high energy secondary neutrons, protons, and α-particles. Some of these fragments may therefore be scattered almost isotropically [11]-[12]. In the case of a high energy proton beam, the dose from secondary protons is dominating in comparison to other secondaries, cf [13]. The bipartition model for ion transport, under continuously slowing down approximation, 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 cut off angle were treated with the straight forward ion group and thus separated from those protons of more diffusive character. The bipartition model here, illustrated with the SHIELD-HIT+ MC simulations. The results are discussed in the aspect of the primary particles flunce, planar fluence and absorbed dose of primary H^1 ions and their associated H^1 fragments in tissue-like media with ranges of clinical interest.

The *Monte Carlo SHIELD-HIT+ code* has advantageous features for implementing radiation for charged particles, see [14]-[15]. Following the therapeutic ranges above, we calculate the depth absorbed dose distribution of 70MeV/u and 202 MeV/u 1H ion beams. 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 center of a cylindrical water phantom (R = 10 cm, 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. The energies of the projectiles were chosen to correspond to ranges of approximately 40 and 260 mm in water. In the plots below the dose represented by $D(z)$ corresponds to $D(x)$ in (5.22) and $\Phi(z)$ to the dept fluence $f(x)$. The plots show helium, proton radiation particles of forward directed ion groups and their secondaries for both $70MeV/u\, H^1$ and $202MeV/u\, H^1$ ion beam in water. For Detailed studies and further results of the this type we refer to [13]- [15].

6.1. **Summary.** We give 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 single- and multi-layer 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 MC method suitable for computations in therapeutic applications.

The results are in Fig. 1 and 2 that we concisely describe below: in Fig 1. The curves have been normalized to the respective values of the different transport parameters at the phantom surface, z = 0. The dominated forward directed protons are given by the sum of the primary and secondary protons associated planar components. The diffusion related ion group is closely related to the transport of secondaries Cf. Fig. 2. In Fig. 2. 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 part in the discussed bipartition model.

To conclude it is clear that in the therapeutic, the fluence of high energy proton beam, in the forward directed particles, is both related to the transport of primary 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. [15]. The bi-partition model, with retained energy straggling term, could then be a compliment to other particle transport models to identify the, more isotropically scattered generated, secondary protons in therapeutic high energy proton beams.

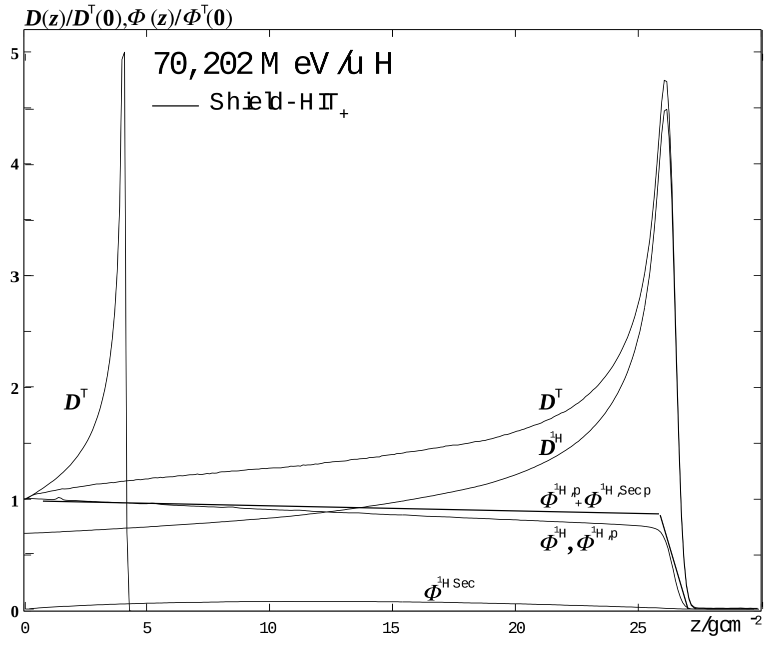

Fig. 1 SHIELD-HIT+ MC simulation of the total absorbed dose D^T, fulence Φ, planer fulence Φ^P of the primary and secondary protons generated in a therapeutic $202 MeV/u\, H^1$ ion beam in water. The curves are normalized to the respective values of the different transport parameters at the phantom surface, z = 0.

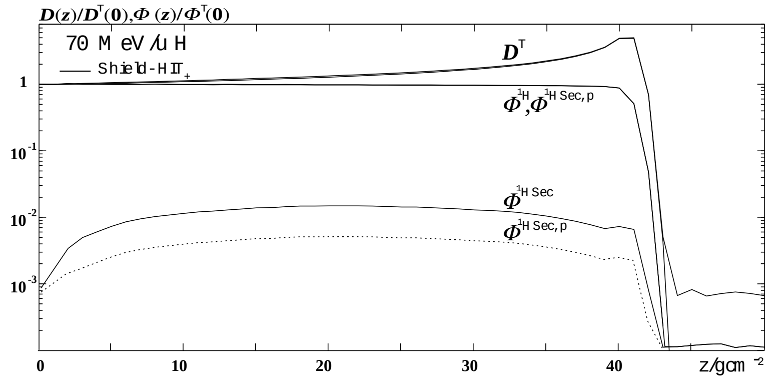

Fig. 2 A close up of the total absorbed dose D^T, fluence Φ, planar fluence Φ^P of the primary and secondary protons generated in a therapeutic $70MeV/u\, H^1$ ion beam in water using SHIELD-HIT+ MC simulations. The curves have been normalized to the respective values of the different transport parameters at the phantom surface, z = 0.

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