Comparison between radiative transfer theory and the simplified spherical harmonics approximation for a semi-infinite geometry

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In this study, the third-order simplified spherical harmonics equations (SP_3), an approximation of the radiative transfer equation, are solved for a semi-infinite geometry considering the exact simplified spherical harmonics boundary conditions. The obtained Green's function is compared to radiative transfer calculations and the diffusion theory. In general, it is shown that the SP_3 equations provide better results than the diffusion approximation in media with high absorption coefficient values but no improvement is found for small distances to the source.

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The simplified spherical harmonics equations (SP_N equations), an approximation of the radiative transfer equation (RTE), were recently introduced in the field of biomedical optics [1]. In the past years, the SP_N approximation has aroused increasing interest [2,3] because the application of the conventional diffusion approximation leads in many cases to unsatisfying results. Furthermore, the use of these coupled diffusionlike equations together with the corresponding boundary conditions (BCs) avoids the high computational complexity of the conventional spherical harmonics method (P_N method) [1,4]. However, in literature, solutions of the SP_N equations for boundary-value problems have up to now been based only on numerical methods, such as the finite difference method [5], the finite volume method [3], or the finite element method [6–8]. In contrast to numerical methods, analytical approaches are, in general, exact, fast to evaluate, and usable for validation of the numerical results. Recently, the infinite space Green's function for the SP_3 and SP_5 equations was derived and compared to solutions of the RTE [9].

In this Letter we present the solution of the SP_3 equations for the boundary-value problem of a semi-infinite geometry assuming a source distribution inside the medium. The obtained Green's function is compared with radiative transfer calculations and the diffusion equation (DE). The Monte Carlo (MC) method is applied for solving the RTE [10].

The third-order simplified spherical harmonics equations in the steady-state domain are given by the following system of two coupled partial differential equations [1]:

$$-\nabla\frac{1}{3\sigma_1}\nabla\varphi_1(\mathbf{r})+\sigma_0\varphi_1(\mathbf{r})=S(\mathbf{r})+\frac{2}{3}\sigma_0\varphi_2(\mathbf{r}),$$
$$-\nabla\frac{1}{7\sigma_3}\nabla\varphi_2(\mathbf{r})+\left(\frac{4}{9}\sigma_0+\frac{5}{9}\sigma_2\right)\varphi_2(\mathbf{r})=-\frac{2}{3}S(\mathbf{r})+\frac{2}{3}\sigma_0\varphi_1(\mathbf{r}), \tag{1}$$

where $\varphi_i(\mathbf{r})$, $i=1,2$, are the composite moments of the radiance, $\sigma_n=\mu_a+\mu_s(1-f_n)$ are the absorption coefficients of order n, $S(\mathbf{r})$ is the internal light source density, μ_s is the scattering coefficient, and f_n are the corresponding expansion coefficients of a rotationally invariant phase function that is expanded in Legendre polynomials $P_n(x)$ and defined as

$$f_n=2\pi\int_{-1}^{1}f(\mu)P_n(\mu)\mathrm{d}\mu. \tag{2}$$

In the case of the Henyey–Greenstein function, they become $f_n=g^n \quad \forall\, n\in\mathbb{N}_0$, where $g=\langle\mu\rangle$. For obtaining the Green's function of these equations in a semi-infinite geometry, an isotropic emitting point source $S(\mathbf{r})=\delta(\mathbf{r}-\mathbf{r}')$, which is placed along the positive z axis at $z=z'$, is considered. Expanding the composite moments and the source distribution in the form of the zero-order Hankel transform,

$$\varphi_i(\mathbf{r})=\frac{1}{2\pi}\int_0^\infty\varphi_i(q,z)J_0(q\rho)q\mathrm{d}q, \tag{3}$$

$$\delta(\mathbf{r}-\mathbf{r}')=\frac{\delta(z-z')}{2\pi}\int_0^\infty J_0(q\rho)q\mathrm{d}q, \tag{4}$$

where $J_0(x)$ is the zeroth-order Bessel function of the first kind, yields a system of second-order differential equations for $\psi=[\varphi_1(q,z),\varphi_2(q,z)]^T$:

$$\frac{d^2\psi}{dz^2}=(\mathbf{A}+q^2\mathbf{I}_2)\psi+\delta(z-z')\varepsilon, \tag{5}$$

with the coefficient matrix

$$\mathbf{A}=\begin{pmatrix}3\sigma_0\sigma_1 & -2\sigma_0\sigma_1\\ -\frac{14}{3}\sigma_0\sigma_3 & \frac{28}{9}\sigma_0\sigma_3+\frac{35}{9}\sigma_2\sigma_3\end{pmatrix} \tag{6}$$

and the vector

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$$\varepsilon = \frac{1}{3}\begin{pmatrix} -9\sigma_1 \\ 14\sigma_3 \end{pmatrix}. \tag{7}$$

The matrix $\mathbf{I}_2 = \mathrm{diag}(1,1)$ equals the identity matrix. Regarding the source free domain, we seek a solution in the form of plane wave modes:

$$\psi(q,z) = e^{\lambda z}|\nu\rangle, \tag{8}$$

where λ and $|\nu\rangle$ denote the corresponding eigenvalue and eigenvector. The matrix $\mathbf{A}$ has two real-valued eigenvalues and can be written in the form $\mathbf{A} = \mathcal{B}\mathcal{D}\mathcal{B}^{-1}$, where $\mathcal{B}$ is the transformation matrix that contains the eigenvectors of $\mathbf{A}$ and $\mathcal{D} = \mathrm{diag}(\xi_1^2, \xi_2^2)$. The eigenvalues of the equation $\det(\mathbf{A} - \xi^2\mathbf{I}_2) = 0$ are given by

$$\xi_{1/2}^2 = \alpha \pm \sqrt{\alpha^2 - \beta}, \tag{9}$$

where the constants become

$$\alpha = \frac{3}{2}\sigma_0\sigma_1 + \frac{28}{18}\sigma_0\sigma_3 + \frac{35}{18}\sigma_2\sigma_3, \quad \beta = \frac{35}{18}3\sigma_0\sigma_1\sigma_2\sigma_3. \tag{10}$$

The resulting eigenvalue problem can be written as

$$[\mathcal{D} - (\lambda^2 - q^2)\mathbf{I}_2]\cdot\mathcal{B}^{-1}|\nu\rangle = 0, \tag{11}$$

where the q-dependent and positive eigenvalues are obtained as

$$\lambda_1(q) = \sqrt{q^2 + \xi_1^2}, \qquad \lambda_2(q) = \sqrt{q^2 + \xi_2^2}. \tag{12}$$

The q-independent eigenvectors become

$$|\nu_i\rangle = \begin{pmatrix} 2\sigma_0\sigma_1 \\ 3\sigma_0\sigma_1 - \xi_i^2 \end{pmatrix}. \tag{13}$$

Thus, the homogeneous solution that satisfies the BCs for the semi-infinite geometry $\psi(q,z) \to 0$ for $z \to \infty$ is obtained as

$$\psi^{(h)}(q,z) = \mathcal{C}_1(q)|\nu_1\rangle e^{-\lambda_1(q)z} + \mathcal{C}_2(q)|\nu_2\rangle e^{-\lambda_2(q)z}. \tag{14}$$

For finding the infinite space Green's function, the following plane wave decompositions,

$$\varphi_i(q,z) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\varphi_i(q,k)e^{-jkz'}e^{jkz}\mathrm{d}k, \qquad \delta(z-z') = \frac{1}{2\pi}\int_{-\infty}^{\infty}e^{-jkz'}e^{jkz}\mathrm{d}k \tag{15}$$

are considered. Inserting these integral representations into the system in Eq. (5) leads to a system of linear equations:

$$[\mathbf{A} + (q^2 + k^2)\mathbf{I}_2]\psi^{(p)}(q,k) = -\varepsilon. \tag{16}$$

The composite moments in Fourier space are obtained as

$$\psi^{(p)}(q,k) = \frac{H_1|\nu_1\rangle}{k^2 + \lambda_1^2(q)} - \frac{H_2|\nu_2\rangle}{k^2 + \lambda_2^2(q)}, \tag{17}$$

with constants

$$H_1 = \frac{14\sigma_3\langle 1|\nu_2\rangle + 9\sigma_1\langle 2|\nu_2\rangle}{3|A|},$$
$$H_2 = \frac{14\sigma_3\langle 1|\nu_1\rangle + 9\sigma_1\langle 2|\nu_1\rangle}{3|A|}. \tag{18}$$

The evaluation of the inverse Fourier integrals in Eq. (15) yields the free space Green's function:

$$\psi^{(p)}(q,z) = \frac{H_1|\nu_1\rangle}{2}\frac{\exp(-\lambda_1(q)|z-z'|)}{\lambda_1(q)}, \tag{19}$$

$$-\frac{H_2|\nu_2\rangle}{2}\frac{\exp(-\lambda_2(q)|z-z'|)}{\lambda_2(q)}. \tag{20}$$

Thus, the general solution of the boundary-value problem in the transformed space is given via superposition:

$$\psi(q,z) = \psi^{(h)}(q,z) + \psi^{(p)}(q,z). \tag{21}$$

Now, the exact BC within the SP_N approximation [1] at the plane $z = 0$ with the outward normal vector $\mathbf{n} = -\hat{\mathbf{z}}$

$$\left(\frac{1}{2} + A_1\right)\varphi_1(q,0) - \frac{1+B_1}{3\sigma_1}\frac{d\varphi_1(q,z)}{dz}\bigg|_{z=0} = \left(\frac{1}{8} + C_1\right)\varphi_2(q,0) - \frac{D_1}{\sigma_3}\frac{d\varphi_2(q,z)}{dz}\bigg|_{z=0}, \tag{22}$$

$$\left(\frac{7}{24} + A_2\right)\varphi_2(q,0) - \frac{1+B_2}{7\sigma_3}\frac{d\varphi_2(q,z)}{dz}\bigg|_{z=0} = \left(\frac{1}{8} + C_2\right)\varphi_1(q,0) - \frac{D_2}{\sigma_1}\frac{d\varphi_1(q,z)}{dz}\bigg|_{z=0} \tag{23}$$

can be implemented. The corresponding constants $(A_1, B_1, \ldots)$ are explicitly given in the appendix of [1]. This task involves the solution of a simple system of two linear equations for determination of the q-dependent constants $\mathcal{C}_1(q)$ and $\mathcal{C}_2(q)$. We omit this calculation step here. After this procedure, the solution for the composite moments in a semi-infinite geometry is obtained as

$$\psi(\mathbf{r}) = H_1|\nu_1\rangle\frac{\exp(-\xi_1\sqrt{\rho^2 + (z-z')^2})}{4\pi\sqrt{\rho^2 + (z-z')^2}}, \tag{24}$$

$$-H_2|\nu_2\rangle\frac{\exp(-\xi_2\sqrt{\rho^2 + (z-z')^2})}{4\pi\sqrt{\rho^2 + (z-z')^2}}, \tag{25}$$

$$+\frac{1}{2\pi}\int_0^{\infty}\psi^{(h)}(q,z)J_0(q\rho)q\mathrm{d}q. \tag{26}$$

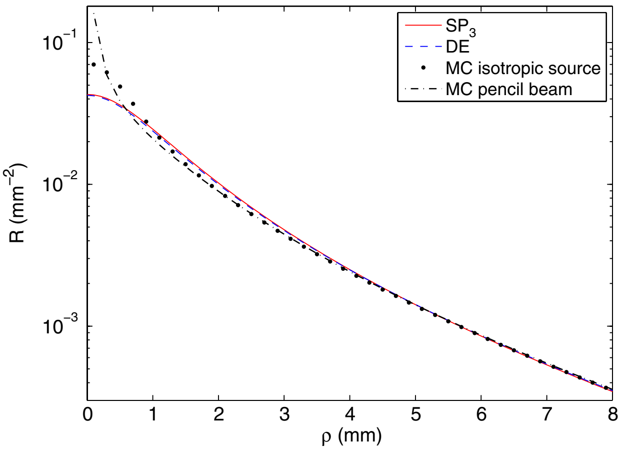

Fig. 1. (Color online) Comparison of the steady-state reflectance versus radial distance ρ for a semi-infinite geometry with optical properties of $\mu_a = 0.01\,\text{mm}^{-1}$ and $\mu_s = 10\,\text{mm}^{-1}$.

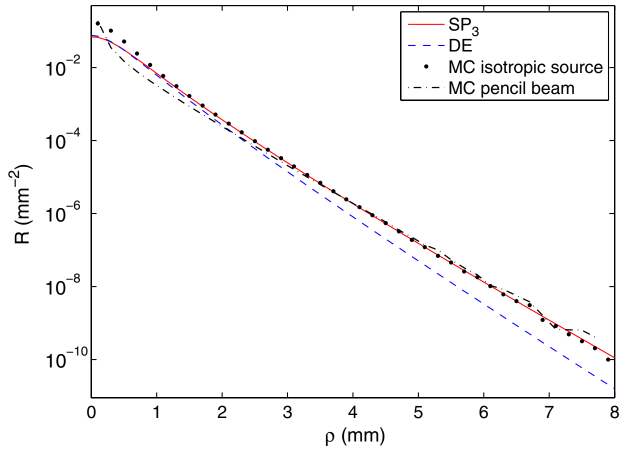

Fig. 2. (Color online) Comparison of the steady-state reflectance versus radial distance ρ for a semi-infinite geometry with optical properties of $\mu_a = 1\,\text{mm}^{-1}$ and $\mu_s = 10\,\text{mm}^{-1}$.

The fluence $\Phi(\mathbf{r})$ and the reflectance $R(\rho)$ at the boundary $z = 0$ in the SP_3 approximation are given by

$$\Phi(\mathbf{r}) = \varphi_1(\mathbf{r}) - \frac{2}{3}\varphi_2(\mathbf{r}), \tag{27}$$

$$R(\rho) = \left(\frac{1}{4} + J_0\right)\left(\varphi_1 - \frac{2}{3}\varphi_2\right) + \frac{1 + 2J_1}{6\sigma_1}\frac{d\varphi_1}{dz} + \left(\frac{5}{16} + J_2\right)\frac{\varphi_2}{3} + \frac{J_3}{7\sigma_3}\frac{d\varphi_2}{dz}, \tag{28}$$

where the values of the constants $(J_0, J_1, \ldots)$ are also explicitly given in [1]. Note that, in the steady-state domain, the SP_1 approximation equals the DE combined with the partial-current-boundary condition (PCBC). An analytical solution to the DE for a semi-infinite geometry under the PCBC can be obtained from [11].

For the following comparisons, we applied for all theories an isotropically emitting point source that is placed at $z' = l^*$, where $l^* = 1/\sigma_1$ is the transport mean free path. Further, the Henyey–Greenstein phase function with an anisotropic factor $g = 0.9$ is applied. The refractive indices of the nonscattering external area and for the scattering semi-infinite area are chosen as $n_e = 1.0$ and $n = 1.4$, respectively.

Figure 1 shows a comparison between the reflectance from the semi-infinite medium obtained from the MC method, the SP_3 equations, and the diffusion theory for typical optical properties in the IR range. Additionally, the MC simulation for a perpendicular incident beam is shown. It can be seen that the SP_3 equations and the DE lead to almost the same reflectance because the absorption coefficient is relatively small. The well-known breakdown of the diffusion theory for small source detector distances cannot be eliminated by using the coupled equations. It is worth mentioning that the application of the extrapolated BCs instead of the more complicated SP_N BC gives better agreement to the radiative transfer theory using the Henyey–Greenstein function as the phase function. Next, a similar comparison is performed for a higher absorbing medium. The results are shown in Fig. 2. For higher absorbing media, the reflectance obtained from the SP_3 equations agrees better with the MC simulation for large distances compared to the solutions of the diffusion theory. However, at small distances to the isotropic point, again, no improvements can be seen.

In conclusion, we derived an analytical solution of the SP_3 equations for a semi-infinite medium, applying the exact BCs. We showed that, for large absorption coefficients, the newly derived solution agrees much better with MC simulations compared to diffusion theory, except for small distances to the source. The derived solution can also be used for applications in the time domain by introducing complex absorption coefficients and using the Fourier transform.

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