Analytical solutions of the simplified spherical harmonics equations

Andre Liemert and Alwin Kienle*
Institut für Lasertechnologien in der Medizin und Messtechnik, Helmholtzstrasse 12, D-89081 Ulm, Germany
**Corresponding author: alwin.kienle@ilm.uni-ulm.de*

Received August 18, 2010; accepted September 21, 2010;
posted September 28, 2010 (Doc. ID 133633); published October 14, 2010

We derived analytical solutions of the simplified spherical harmonics equations, an approximation of the radiative transfer equation, for infinitely extended scattering media. The derived equations are simple (sum of exponential functions) and quickly evaluated. We compared the solutions with Monte Carlo simulations in the steady-state and time domains and found much better agreement compared to solutions of the diffusion equation, especially for large absorption coefficients, short time values, and small distances from the source.
OCIS codes: 170.0170, 170.3660, 010.5620, 290.1990, 290.7050.

The spherical harmonics equations (SP_N) [1] are an approximation of the radiative transfer equation [2,3] for calculation of light propagation in scattering media. Originally, these equations were used for simulation of neutron transport in nuclear sciences [4]. Recently, the equations were introduced in the field of biomedical optics, where they have been solved using numerical methods [1,5,6].

In this Letter we present for the first time, to the best of our knowledge, analytical solutions of the SP_N equations. In particular, the Green's functions of the SP_3 and SP_5 equations for infinitely extended scattering media are derived in the steady-state and in the frequency domains. The time domain solutions are obtained by applying the Fourier transform.

The SP_3 simplified spherical harmonics equations in the steady-state domain are given by the following system of coupled partial differential equations [1]:

$$\begin{aligned}&-\nabla\frac{1}{3\mu_{a1}}\nabla\varphi_1(\vec{r})+\mu_a\varphi_1(\vec{r})=S(\vec{r})+\frac{2}{3}\mu_a\varphi_2(\vec{r}),\\&-\nabla\frac{1}{7\mu_{a3}}\nabla\varphi_2(\vec{r})+\left(\frac{4}{9}\mu_a+\frac{5}{9}\mu_{a2}\right)\varphi_2(\vec{r})\\&=-\frac{2}{3}S(\vec{r})+\frac{2}{3}\mu_a\varphi_1(\vec{r}),\end{aligned}\tag{1}$$

where $\varphi_i(\vec{r})$ $(i=1,2)$ are the composite moments of the radiance, $\mu_{an}=\mu_a+\mu_s(1-g^n)$ are the absorption coefficients of order n, g is the anisotropy factor, and μ_s is the scattering coefficient [1]. The absorption coefficient of order zero equals the normally defined absorption coefficient μ_a, $S(\vec{r})$ is the internal light source density, and the reduced scattering coefficient is given by $\mu_s'=\mu_s(1-g)$. The relation

$$\varphi(r)=\frac{1}{2\pi^2 r}\int_0^\infty k\varphi(k)\sin(kr)\mathrm{d}k,\tag{2}$$

which corresponds to the three-dimensional Fourier transform for the spherically symmetric case, is used to represent the composite moments by plane waves. The Green's function of Eq. (1) is obtained by setting $S(\vec{r})=\delta(r)/(4\pi r^2)$; i.e., an isotropically emitting point source is assumed. The plane wave expansion of the source is given by

$$S(r)=\frac{1}{2\pi^2 r}\int_0^\infty k\sin(kr)\mathrm{d}k.\tag{3}$$

Inserting the integral representations [Eqs. (2) and (3)] in the SP_3 equations [Eq. (1)] results in a system of linear equations:

$$\begin{pmatrix}\frac{k^2}{3\mu_{a1}}+\mu_a & -\frac{2}{3}\mu_a\\ -\frac{2}{3}\mu_a & \frac{k^2}{7\mu_{a3}}+\frac{4}{9}\mu_a+\frac{5}{9}\mu_{a2}\end{pmatrix}\begin{pmatrix}\varphi_1(k)\\ \varphi_2(k)\end{pmatrix}=\begin{pmatrix}1\\ -\frac{2}{3}\end{pmatrix}.\tag{4}$$

The composite moments φ_i $(i=1,2)$ are determined as

$$\varphi_i(k)=\frac{F_i^{(1)}(k^2)}{k^4+\alpha k^2+\beta},\qquad F_i^{(m)}(x)=\sum_{j=i-1}^{m}a_{ij}x^j,\tag{5}$$

where the functions $F_i^{(m)}(x)$ are defined for a compact notation of the results. The coefficients for the polynomials of the numerators are

$$a_{10}=\frac{35}{3}\mu_{a1}\mu_{a2}\mu_{a3},\qquad a_{11}=3\mu_{a1},\qquad a_{21}=-\frac{14}{3}\mu_{a3},\tag{6}$$

and those for the polynomial of the denominator are

$$\begin{aligned}\alpha&=3\mu_a\mu_{a1}+\frac{28}{9}\mu_a\mu_{a3}+\frac{35}{9}\mu_{a2}\mu_{a3},\\ \beta&=\frac{35}{3}\mu_a\mu_{a1}\mu_{a2}\mu_{a3}.\end{aligned}\tag{7}$$

Next, the zeros of the polynomial $Q(\lambda)=\lambda^2+\alpha\lambda+\beta$ are determined. Note that the coefficients α and β are real and positive numbers. Such a polynomial is called a Hurwitz polynomial [7]. The zeros $\lambda_{1,2}=(-\alpha\pm\sqrt{\alpha^2-4\beta})/2$ are located in the left half-plane of the complex plane. Further, it can be shown that the discriminant $\mathcal{D}=\alpha^2-4\beta$ of the equation $Q(\lambda)=0$ is always positive. Next, the composite moments are split in partial fractions. An appropriate ansatz is made by

$$\varphi_i(k) = \frac{F_i^{(1)}(k^2)}{(k^2+k_1^2)(k^2+k_2^2)} = \frac{A_i}{k^2+k_1^2} + \frac{B_i}{k^2+k_2^2}, \tag{8}$$

where $k_1 = \sqrt{-\lambda_1}$ and $k_2 = \sqrt{-\lambda_2}$. The coefficients are determined as

$$A_i = \frac{F_i^{(1)}(\lambda_1)}{k_2^2 - k_1^2}, \qquad B_i = \frac{F_i^{(1)}(\lambda_2)}{k_1^2 - k_2^2}. \tag{9}$$

The infinite space Green's function of the steady-state diffusion equation expressed by plane waves is given as

$$G(r) = \frac{e^{-\mu_{\mathrm{eff}} r}}{4\pi D r} = \frac{1}{2\pi^2 D r}\int_0^\infty \frac{k \sin(kr)}{k^2+\mu_{\mathrm{eff}}^2}\mathrm{d}k, \tag{10}$$

where $D = (3(\mu_s' + \mu_a))^{-1}$ is used as the diffusion coefficient in the steady-state domain and $\mu_{\mathrm{eff}} = \sqrt{3\mu_a(\mu_a + \mu_s')}$ is the effective attenuation coefficient. We note that, for the comparison in the time domain, we use $D = (3\mu_s')^{-1}$. The different diffusion coefficients are applied to better match the results from the diffusion equation compared to Monte Carlo simulations. They do not concern the SP_N solutions.

By comparing Eq. (10) with Eq. (2) using Eq. (8), it can be seen that the composite moments of SP_3 are, in principle, a superposition of two diffusion Green's functions. Thus, we obtain for the composite moments

$$\varphi_i(r) = A_i\frac{e^{-k_1 r}}{4\pi r} + B_i\frac{e^{-k_2 r}}{4\pi r}, \qquad i = 1, 2. \tag{11}$$

The total fluence rate is a combination of the two composite moments [1]:

$$\psi(r) = \varphi_1(r) - \frac{2}{3}\varphi_2(r). \tag{12}$$

The procedure for obtaining an analytical solution for the SP_5 equations is equal to the SP_3 case shown above. By applying Eq. (2) to the system of three ordinary differential equations, given by Klose and Larsen [1], we get a system of linear equations for the composite moments $\varphi_i(k)$ ($i = 1, 2, 3$). They are determined as

$$\varphi_i(k) = \frac{F_i^{(2)}(k^2)}{k^6 + \alpha k^4 + \beta k^2 + \gamma}, \tag{13}$$

with the coefficients of the numerators

$$\begin{aligned}
a_{10} &= \frac{231}{5}\mu_{a1}\mu_{a2}\mu_{a3}\mu_{a4}\mu_{a5},\\
a_{11} &= \frac{35}{3}\mu_{a1}\mu_{a2}\mu_{a3} + 33\mu_{a1}\mu_{a5}\left(\frac{16}{45}\mu_{a2} + \frac{9}{25}\mu_{a4}\right),\\
a_{12} &= 3\mu_{a1}, \qquad a_{21} = -\frac{462}{25}\mu_{a3}\mu_{a4}\mu_{a5},\\
a_{22} &= -\frac{14}{3}\mu_{a3}, \qquad a_{32} = \frac{88}{15}\mu_{a5},
\end{aligned} \tag{14}$$

and of the denominator

$$\begin{aligned}
\alpha &= 3\mu_a\mu_{a1} + \frac{28}{9}\mu_a\mu_{a3} + \frac{35}{9}\mu_{a2}\mu_{a3}\\
&\quad + 11\mu_{a5}\left(\frac{64}{225}\mu_a + \frac{16}{45}\mu_{a2} + \frac{9}{25}\mu_{a4}\right),\\
\beta &= \mu_a\mu_{a1}\left(\frac{35}{3}\mu_{a2}\mu_{a3} + \frac{176}{15}\mu_{a2}\mu_{a5} + \frac{297}{25}\mu_{a4}\mu_{a5}\right)\\
&\quad + \mu_{a3}\mu_{a4}\mu_{a5}\left(\frac{308}{25}\mu_a + \frac{77}{5}\mu_{a2}\right),\\
\gamma &= \frac{231}{5}\mu_a\mu_{a1}\mu_{a2}\mu_{a3}\mu_{a4}\mu_{a5}.
\end{aligned} \tag{15}$$

The zeros of the polynomial $Q(\lambda) = \lambda^3 + \alpha\lambda^2 + \beta\lambda + \gamma$ can be found by using Cardano's formula [7]. By setting

$$p = \frac{1}{3}\alpha^2 - \beta, \qquad q = \frac{2}{27}\alpha^3 - \frac{1}{3}\alpha\beta + \gamma, \tag{16}$$

and using the following expression for $k = 0, 1, 2$:

$$\lambda_{k+1} = 2\sqrt{\frac{p}{3}}\cos\left(\frac{\varphi + 2k\pi}{3}\right) - \frac{\alpha}{3}, \tag{17}$$

where

$$\varphi = \arccos\left(-\frac{3q}{2p}\sqrt{\frac{3}{p}}\right), \tag{18}$$

the roots of $Q(\lambda)$ are obtained. Similar to the SP_3 case, the Hurwitz criterion gives the following result for the location of the zeros: $\mathrm{Re}\{\lambda_{k+1}\} < 0$. The moments for the SP_5 equations are given by

$$\varphi_i(r) = A_i\frac{e^{-k_1 r}}{4\pi r} + B_i\frac{e^{-k_2 r}}{4\pi r} + C_i\frac{e^{-k_3 r}}{4\pi r}, \qquad i = 1, 2, 3, \tag{19}$$

with the coefficients

$$\begin{aligned}
A_i &= \frac{F_i^{(2)}(\lambda_1)}{(k_2^2 - k_1^2)(k_3^2 - k_1^2)}, \qquad B_i = \frac{F_i^{(2)}(\lambda_2)}{(k_1^2 - k_2^2)(k_3^2 - k_2^2)},\\
C_i &= \frac{F_i^{(2)}(\lambda_3)}{(k_1^2 - k_3^2)(k_2^2 - k_3^2)}.
\end{aligned} \tag{20}$$

For the SP_5 equations, the total fluence rate is defined as [1]

$$\psi(r) = \varphi_1(r) - \frac{2}{3}\varphi_2(r) + \frac{8}{15}\varphi_3(r). \tag{21}$$

The SP_N equations in the frequency domain are obtained from the steady-state domain version for SP_5 by setting $\mu_{an} = \mu_a + \mu_s(1 - g^n) + j\omega/c$, where ω is the angular frequency of the intensity modulated light, c is the speed of light, and $j = \sqrt{-1}$. The time-dependent solution is found by performing the inverse Fourier transform. We note that, for the SP_1 approximation, it is possible to derive an analytical formula directly in the time domain.

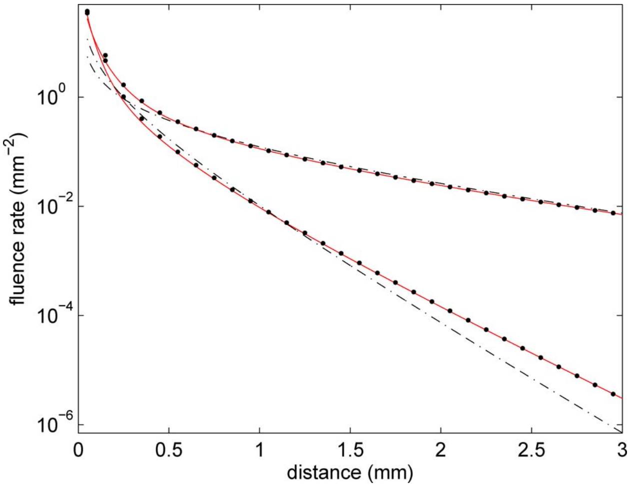

Fig. 1. (Color online) Steady-state fluence rate versus distance from the isotropic source for an infinite scattering medium. The optical parameters are $\mu_s' = 1\ \mathrm{mm}^{-1}$, $g = 0.9$, $\mu_a = 0.2\ \mathrm{mm}^{-1}$ (upper curves), and $\mu_a = 2\ \mathrm{mm}^{-1}$ (lower curves).

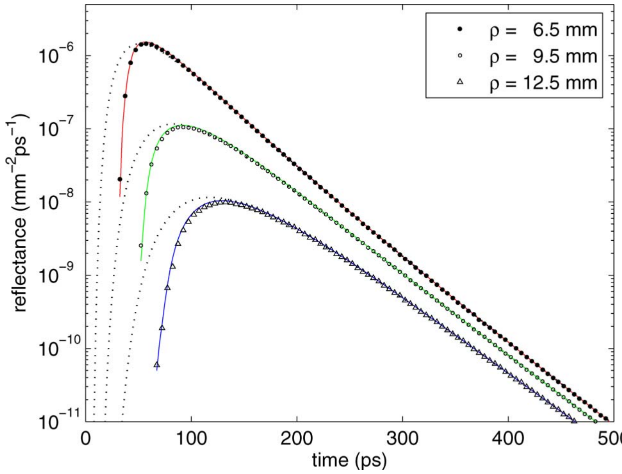

Fig. 2. (Color online) Time resolved reflectance from a semi-infinite scattering medium. The optical properties are $\mu_s' = 1\ \mathrm{mm}^{-1}$, $g = 0.9$, and $\mu_a = 0.1\ \mathrm{mm}^{-1}$. A refractive index of 1.0 and 1.4 was used outside and inside the scattering medium.

We compared the derived solutions with (a) Monte Carlo simulations [8], which are, in the limit of an infinitely large number of simulated photons, an exact solution of the radiative transport equation, and (b) the often used diffusion approximation [2]. The Henyey–Greenstein function was used as phase function in the Monte Carlo simulations. Figure 1 shows the fluence rate versus distance from the isotropic point source for $\mu_s' = 1\ \mathrm{mm}^{-1}$, $g = 0.9$, $\mu_a = 0.2\ \mathrm{mm}^{-1}$ (upper curves), and $2\ \mathrm{mm}^{-1}$ (lower curves) calculated with SP_5 [Eq. (21), solid curves], the diffusion approximation [Eq. (10), dashed curves], and the Monte Carlo method (dotted curves). We note that results obtained from the SP_3 solutions (not shown) are very close to those of the SP_5 solutions given in Fig. 1.

Figure 2 shows the time resolved reflectance from a semi-infinite scattering medium at distances of 6.5, 9.5, and 12.5 mm from the perpendicular incident pencil beam. The solution of the SP_3 equations (solid curves) is shown in comparison with Monte Carlo simulations (symbols) and the solution of the diffusion equation (dotted curves). The reflectance was calculated with the method of image sources using the extrapolated boundary conditions; see Eq. 7 in [8].

The figures show that the SP_N solutions are very close to the results obtained from the Monte Carlo simulations. The diffusion theory, however, performs much worse. In the steady-state domain in case of $\mu_a = 0.2\ \mathrm{mm}^{-1}$, diffusion theory is valid only for large distances from the source, whereas for small distances or for large absorption coefficients, it fails to describe light propagation in scattering media. In the time domain, the SP_N solutions describe the light propagation even for very short time values, where diffusion theory breaks down.

In conclusion, analytical solutions of the SP_3 and SP_5 equations were derived for infinitely large scattering media. We showed that these solutions are very close to results obtained by solving the radiative transfer equation even for large absorption coefficients, small time values, and short distances from the isotropic δ-source. For example, in biomedical optics, absorption coefficients in the range of $\mu_a \approx 1\ \mathrm{mm}^{-1}$ are typical in the blue or green wavelength range, and thus a correct description of light propagation for this case is of great importance. Similarly, in the time domain, the photons detected at small distances and early time values were often neglected owing to failure of the diffusion approximation, although they contain important information [9]. The derived solutions consist only of exponential functions and are therefore easily programmed and quickly evaluated.

The authors thank Alexander Klose for turning our attention to the analytical solution of the SP_3 equations.

References

1. A. D. Klose and E. W. Larsen, J. Comput. Phys. **220**, 441 (2006).
2. A. Ishimaru, *Wave Propagation and Scattering in Random Media* (Academic, 1978).
3. H. Xu and M. S. Patterson, Phys. Med. Biol. **51**, N247 (2006).
4. P. S. Brantley and E. W. Larsen, Nucl. Sci. Eng. **134**, 1 (2000).
5. M. Chu, K. Vishwanath, A. D. Klose, and H. Dehghani, Phys. Med. Biol. **54**, 2493 (2009).
6. J. Bouza-Domínguez, Y. Bérubé-Lauzière, and V. Issa, Appl. Opt. **49**, 1414 (2010).
7. T. Frey and M. Bossert, *Signal- und Systemtheorie* (B. G. Teubner, 2004).
8. A. Kienle and M. S. Patterson, J. Opt. Soc. Am. A **14**, 246 (1997).
9. A. Pifferi, A. Torricelli, L. Spinelli, D. Contini, R. Cubeddu, F. Martelli, G. Zaccanti, A. Tosi, A. D. Mora, F. Zappa, and S. Cova, Phys. Rev. Lett. **100**, 138101 (2008).