Hybrid diffusion approximation in highly absorbing media and its effects of source approximation

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A modified diffusion approximation model called the hybrid diffusion approximation that can be used for highly absorbing media is investigated. The analytic solution of the hybrid diffusion approximation for reflectance in two-source approximation and steady-state case with extrapolated boundary is obtained. The effects of source approximation on the analytic solution are investigated, and it is validated that two-source approximation in highly absorbing media to describe the optical properties of biological tissue is necessary. Monte Carlo simulation of recovering optical parameters from reflectant data is done with the use of this model. The errors of recovering μ_a and μ'_s are smaller than 15% for the reduced albedo between 0.77 and 0.5 with the source-detector separation of 0.4–3 mm.

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With the development of biomedical optical technology, the determination of optical parameters of biological tissue is becoming one of the most important basic research topics^[1,2], and the diffusion reflectance technique which can be used in noninvasive measurement has received a great deal of attention recently [3-5]. The basic principle of the technique is based on the theory model of the relationship between the reflectance and the optical coefficients of biological media, and an inversion algorithm is used to reconstruct the optical properties of the tissue from the obtained reflectance data. The diffusion approximation (DA) is a successful theory for solving the radiative transport equation. However, the DA model is valid only in highly scattering and low absorbing media. A typical criterion is that the reduced albedo $[a' \equiv \mu'_{\rm s}/(\mu_{\rm a} + \mu'_{\rm s})]$ must be higher than $0.9^{[2]}$, where $\mu_{\rm a}$ is the absorption coefficient, $\mu'_{\rm s}$ is the reduced scattering coefficient.

Several researchers have recently adopted different methods to make an extension of the $DA^{[6-10]}$. Venugopalan et al. developed an extension to the DA with a δ -Eddington phase function for highly absorbing infinite media and small source-detector separations^[6]. In the standard DA, the diffusion coefficient $D = 1/[3(\mu_{\rm a} + \mu'_{\rm s})]$, Aronson et al. improved the expression of D and gave a new diffusion coefficient $D_{\text{Aron}} = 1/[3(\alpha \mu_{\text{a}} + \mu'_{\text{s}})]$ for highly absorbing media^[7,8]. Ripoll *et al.* applied D_{Aron} in the standard DA, and showed the validity of this improved diffusion approximation^[9]. Hull et al. studied the steady-state reflectance spectroscopy in P_3 approximation, and proved that a hybrid Green's function had a good agreement with P_3 Green's function^[10]. In this letter, based on this hybrid Green's function, a modified DA model which can be used in highly absorbing media is expatiated, and the effects of source approximation on the spatially resolved diffuse reflectance are investigated.

The P_3 approximation considers the high-order term of

the radiance:

$$L(r, \hat{s}) = \sum_{l=0}^{3} \frac{2l+1}{4\pi} \psi_l(r) P_l(\mathbf{r} \cdot \hat{s}).$$
 (1)

The radiance fluence $\psi_0(r)$ of the Green's function solution in a spherically symmetric is expressed as^[11]

$$\psi_0(r) = C_- Q_0(-\nu_- r) + C_+ Q_0(-\nu_+ r), \qquad (2)$$

where

$$C_{-} = \frac{\nu_{-}^{5}[3\mu_{a}(\mu_{a} + \mu'_{s}) - \nu_{+}^{2}]}{12\pi\mu_{a}^{2}(\mu_{a} + \mu'_{s})(\nu_{+}^{2} - \nu_{-}^{2})},$$

$$C_{+} = \frac{\nu_{+}^{5}[3\mu_{a}(\mu_{a} + \mu'_{s}) - \nu_{-}^{2}]}{12\pi\mu_{a}^{2}(\mu_{a} + \mu'_{s})(\nu_{-}^{2} - \nu_{+}^{2})}, \quad Q_{0}(x) = \frac{\exp(x)}{x},$$

and

$$\nu_{-} = \frac{1}{\sqrt{18}} \left(\beta - \sqrt{\beta^2 - \gamma_{\alpha}} \right)^{\frac{1}{2}},$$

$$\nu_{+} = \frac{1}{\sqrt{18}} \left(\beta + \sqrt{\beta^2 - \gamma_{\alpha}} \right)^{\frac{1}{2}},$$
(3)

where

$$\begin{split} \beta &\equiv 27\mu_{\rm a}(\mu_{\rm a} + \mu_{\rm s}') + 28\mu_{\rm a}(\mu_{\rm a} + \mu_{\rm s}'\delta) \\ +35(\mu_{\rm a} + \mu_{\rm s}'\gamma)(\mu_{\rm a} + \mu_{\rm s}'\delta), \\ \gamma_{\alpha} &\equiv 3780\mu_{\rm a}(\mu_{\rm a} + \mu_{\rm s}')(\mu_{\rm a} + \mu_{\rm s}'\gamma)(\mu_{\rm a} + \mu_{\rm s}'\delta), \\ \gamma &= (1 - g_2)/(1 - g_1), \quad \delta = (1 - g_3)/(1 - g_1), \end{split}$$

and the first-moment $g_1 = g$ is the scattering anisotropy factor, g_2 and g_3 are the second-moment and third-moment of the phase function, respectively.

In Eq. (2), $\psi_0(r)$ consists of two terms, but $\psi_1(r) \neq -\kappa |\nabla \psi_0(r)|$, κ is an arbitrary constant, so $\psi_0(r)$ and $\psi_1(r)$ do not satisfy Fick's law. The flux $\psi_1(r)$ is given by

$$\psi_{1}(r) = -D_{\text{asym}} |\nabla [C_{-}Q_{0}(-\nu_{-}r)]| -D_{\text{trans}} |\nabla [C_{+}Q_{0}(-\nu_{+}r)]|, \qquad (4)$$

that is, each term in Eq. (2) is related by Fick's law to a corresponding team in the flux expression through an associated diffusion coefficient $D_{asym} = \mu_a/\nu_-^2$ and $D_{trans} = \mu_a/\nu_+^2$, where ν_- and ν_+ are the corresponding equivalent attenuation coefficients. The solution associated with ν_+ contributes significantly only at sourcedetector separations of $\rho < 2$ transport mean free paths, therefore, D_{trans} is called as the transient diffusion coefficient. D_{asym} , which has similar tendency with the standard diffusion coefficient D, is called the asymptotic diffusion coefficient^[10]. D_{asym} is approximately equal to D for the high albedo, where DA would be expected to be valid and deviates increasingly from D as the albedo decreases.

The DA only considers the first two terms in Eq. (1), and its Green's function solution of radiance fluence can be expressed as

$$\Phi_0(r) = \frac{1}{4\pi D} \frac{1}{r} \exp\left(-\mu_{\rm eff} r\right),$$
 (5)

where $D = \mu_{\rm a}/\mu_{\rm eff}^2$ is the diffusion coefficient and $\mu_{\rm eff}$ is the equivalent attenuation coefficient. Substituting $D_{\rm asym}$ and ν_{-} for D and $\mu_{\rm eff}$ in Eq. (5), we obtain

$$\Phi_{0,\text{hybrid}}(r) = \frac{1}{4\pi D_{\text{asym}}} \frac{1}{r} \exp\left(-\nu_{-}r\right).$$
(6)

When a pencil beam is incident on a semi-infinite scattering medium along the z axis, the equivalent source is expressed as^[12]

$$q(z) = \frac{a'\mu'_t}{4\pi} \exp(-\mu'_t z), \tag{7}$$

where $\mu'_t = \mu_a + \mu'_s$, the reduced albedo a' is equal to the total integrated source strength because a unit initial beam intensity is assumed. In the standard DA, to satisfy the dipole moment, q(z) is represented as a single point source, which is given as

$$\int_{0}^{\infty} za' \mu'_t \exp(-\mu'_t z) \mathrm{d}z = \int_{0}^{\infty} za' \delta(z - z_0) \mathrm{d}z.$$
(8)

From Eq. (8), we obtain $z_0 = 1/\mu'_t$. To satisfy both the dipole and the quadrupole moments, two point sources are required. Assuming the magnitudes of the two sources are separately equal to a'/2, the sources are given as

$$\int_{0}^{\infty} za' \mu'_{t} \exp(-\mu'_{t}z) dz = \int_{0}^{\infty} za' \frac{1}{2} [\delta(z - z_{01}) + \delta(z - z_{02})] dz, \qquad (9a)$$

$$\int_{0}^{\infty} z^{2}a' \mu'_{t} \exp(-\mu'_{t}z) dz = \int_{0}^{\infty} z^{2}a' \frac{1}{2} [\delta(z - z_{01})] dz$$

$$\int_{0} z^{2} a' \mu'_{t} \exp(-\mu'_{t} z) dz = \int_{0} z^{2} a' \frac{1}{2} [\delta(z - z_{01}) + \delta(z - z_{02})] dz.$$
(9b)



Fig. 1. Approximation for two point sources and its extrapolated boundary condition.

From Eq. (9), we obtain $z_{01} = 2/\mu'_t$ and $z_{02} = 0$, as shown in Fig. 1.

For the extrapolated boundary condition^[13], the fluence is zero at $z_{\rm b} = 2AD_{\rm asym}$, where $A = (1 + R_{\rm eff})/(1 - R_{\rm eff})$ and the effective reflection coefficient $R_{\rm eff}$ is related to the relative refractive index $n_{\rm rel}$ of interface. To satisfy the extrapolated boundary condition $\phi_0 (\rho, z = -z_{\rm b}) = 0$, we must introduce a negative image source at $z = -(2z_{\rm b} + z_0)$ above the tissue surface. The magnitude of the image source is equal to the corresponding real source with an opposite sign. Therefore, for the single point source approximation and two point sources approximation, the source q(z) is respectively expressed as

$$q_{1}(z) = a'\delta(\rho, z - z_{0}) - a'\delta(\rho, z + (2z_{b} + z_{0})), \quad (10)$$

$$q_{2}(z) = \frac{1}{2}a'[\delta(\rho, z - z_{01}) - \delta(\rho, z + (2z_{b} + z_{01})) + \delta(\rho, z - z_{02}) - \delta(\rho, z + (2z_{b} + z_{02}))]. \quad (11)$$

The radiance fluence of the hybrid diffusion approximation can be expressed as $\phi_{0,\text{hybrid}}(\rho, z) = \Phi_{0,\text{hybrid}}(\rho, z) \otimes q(z)^{[14]}$, and the reflectance is given by^[13]

$$R_{\text{hybrid}}(\rho) = \frac{1}{4\pi} \int_{2\pi} \left[1 - R_{\text{Fres}}(\theta) \right] \times \left[\phi_{0,\text{hybrid}}(\rho, z) \Big|_{z=0} + 3D_{\text{asym}} \frac{\partial \phi_{0,\text{hybrid}}(\rho, z)}{\partial z} \Big|_{z=0} \cos \theta \right] \\ \cos \theta d\Omega, \tag{12}$$

where $R_{\text{Fres}}(\theta)$ is the Fresnel reflection coefficient.

To investigate the validity of $R_{\rm hybrid}(\rho)$ in a low albedo medium, $R_{\rm MC}(\rho)$ obtained by the Monte Carlo simulation compiled by Wang *et al.*^[15] is used as the criterion. For comparison, we kept $\mu'_{\rm s} = 1.0 \text{ mm}^{-1}$, n = 1.4, and considered a region of $\rho \leq 10 \text{ mm}$. Henyey-Greenstein phase function with g = 0.9 was used, so the highorder parameters $\gamma = 1.9$ and $\delta = 2.71$. According to the definition of a' and transport mean free path $l'_{\rm t}(l'_{\rm t} \equiv 1/(\mu_{\rm a} + \mu'_{\rm s})), l'_{\rm t}$ is equal to a' numerically. Figure 2 shows the deviation between $R_{\rm hybrid}(\rho)$ and $R_{\rm MC}(\rho)$ defined by $\Delta R/R = |R(\rho) - R_{\rm MC}(\rho)|/R_{\rm MC}(\rho)$.

The influence of the different source approximations on $R_{\rm hybrid}(\rho)$ with $\mu_{\rm a} = 0.01, 0.05, 0.1, 0.5, 0.7, and 1.0$ mm⁻¹ (corresponding to a' = 0.99, 0.95, 0.91, 0.67, 0.59,and 0.5) are provided in Fig. 2. Firstly, it is clearly shown that the percent deviation between $R_{\rm hybrid2}$ and $R_{\rm MC}(\rho)$ is larger than that between $R_{\rm hybrid1}$ and $R_{\rm MC}(\rho)$ for high reduced albedo (as shown in Figs. 2(a)-(c), a' > 0.9) in the region of $0.7l'_t-6l'_t$ close to the source, and the largest deviation from $R_{\rm hybrid2}$ is about 20%;



Fig. 2. Deviation between hybrid diffusion model of single point sources or two point sources approximation (represented by $R_{\text{hybrid1}}(\rho)$ and $R_{\text{hybrid2}}(\rho)$ respectively) and Monte Carlo approximation $R_{\text{MC}}(\rho)$ with different absorption coefficients. (a) $\mu_{\text{a}}=0.01, a'=0.99$; (b) $\mu_{\text{a}}=0.05, a'=0.95$; (c) $\mu_{\text{a}}=0.1, a'=0.91$; (d) $\mu_{\text{a}}=0.5, a'=0.67$; (e) $\mu_{\text{a}}=0.7, a'=0.59$; (f) $\mu_{\text{a}}=1.0, a'=0.5$.

but the error of $R_{hybrid2}$, which decreases with reducing a', is smaller than that of $R_{hybrid1}$ in the region of $6l'_t-10l'_t$ far from the source. Secondly, the deviation of $R_{hybrid1}$ is increasingly large and that of $R_{hybrid2}$ becomes quite small for low reduced albedo (as shown in Figs. 2(d)-(f)) in the region of $0.7l'_t-6l'_t$ close to the source; the difference between $R_{hybrid2}(\rho)$ and $R_{hybrid1}(\rho)$ is small in the region of $6l'_t-10l'_t$ far from the source.

As indicated in the above analysis, the two-source approximation is very necessary for highly absorbing media. The reasons may be due to the fact that one point source of the two-source model is located at the interface ($z_0 = 0$) where single scattered photons have a high probability of escaping and lead the number of the diffuse reflection photons near the source to be reduced so as to make large effect on $R_{\text{hybrid2}}(\rho)$. So the two-source approximation is not always better than one-source approximation, however, the advantage of the two-source model will be increasingly obvious with the increasing of μ_{a} .

In this study, the simulated reflectance $R_{\rm MC}(\rho)$ is used as the experimental data, the nonlinear least-square algorithm is used to fit $R_{\rm MC}(\rho)$ with the two-source hybrid diffusion approximation model $R_{\rm hybrid2}(\rho)$, which is adopted to recover the optical parameters $\mu_{\rm a}$ and $\mu'_{\rm s}$ of the tissue from the reflectance data. The results are shown in Figs. 3 and 4.

Figure 3 clearly shows that the percent deviation between the fitted value and the adopted Monte Carlo simulation value decreases with increasing $\mu_{\rm a}$ for $\mu_{\rm a}$ = 0.01-0.7 mm⁻¹(a' = 0.99-0.59) in the region of ρ = 0.4-3 mm, the deviation is about 27% for $\mu_{\rm a}$ = 0.01 mm⁻¹ and 0.41% for $\mu_{\rm a}$ = 0.7 mm⁻¹. But the deviation shows an increase with the increase of $\mu_{\rm a}$ for $\mu_{\rm a}$ =0.7-1.0 mm⁻¹ (a'=0.59-0.5), the deviation is about 11% for $\mu_{\rm a}$ = 1.0 mm⁻¹, as shown in Fig. 3(b). The results obtained in the region of $\rho = 0.4 - 8$ mm are similar with those in 0.4-3 mm for $\mu_{\rm a}$ =0.1-1.0 mm⁻¹.

The recovery results of the reduced scattering coefficient $\mu'_{\rm s}$ for $\rho = 0.4-8$ mm and 0.4-3 mm are shown in Fig. 4, which clearly shows that the percent deviation between the fitted value and the adopted Monte Carlo simulation value decreases with the increase of $\mu_{\rm a}$ for $\mu_{\rm a} = 0.01-0.5$ mm⁻¹, and the deviation is about 21% for $\mu_{\rm a} = 0.01$ mm⁻¹ and 1.76% for $\mu_{\rm a} = 0.5$ mm⁻¹. And the percent deviation shows an increase with the increase of $\mu_{\rm a}$ for $\mu_{\rm a} = 0.5-1.0$ mm⁻¹, the deviation is about 9.97% for $\mu_{\rm a} = 1.0$ mm⁻¹.

In conclusion, according to the above analysis, the



Fig. 3. (a) Fitted values of $\mu_{\rm a}$ from simulating reflectance data with $\mu_{\rm a}$ = 0.01, 0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, and 1.0 mm⁻¹ by the two-source hybird DA model. The line denotes the exact agreement between fitted and actual absorption coefficients used by Monte Carlo simulation. (b) Deviation between the fitted $\mu_{\rm a}$ and the adopted Monte Carlo simulation $\mu_{\rm a}$.



Fig. 4. Fitted values of $\mu'_{\rm s}$ from simulating reflectance data with $\mu_{\rm a} = 0.01, 0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9,$ and 1.0 mm⁻¹ by the two-source hybird DA model. The horizontal line denotes the value of $\mu'_{\rm s}$ adopted in Monte Carlo simulation. (b) Deviation between the fitted $\mu'_{\rm s}$ and the adopted Monte Carlo simulation $\mu'_{\rm s}$.

spatial resolved diffuse reflectance $R_{\rm hybrid}(\rho)$ of the hybrid diffusion approximation model is suitable for the scattering media with low albedo, and $R_{\rm hybrid}(\rho)$ obtained by the two-source approximation model can be used to describe the distribution of diffuse reflection photons close to the source. As indicated by Monte Carlo simulation experiment, this improved diffusion approximation model can be used for the condition of a' < 0.9, the deviations of $\mu_{\rm a}$ and $\mu'_{\rm s}$ obtained by the two-source approximation are smaller than 15% for a' = 0.77-0.5 in the region of 0.4–3 mm close to the source.

This work is important and useful for developing the technology of diffuse reflection spectral measurement and the theory of radiance measurement, because the reduced albedo a' of biological tissue can be 0.5 or even lower in the visible (400-600 nm) and near infrared (>1000 nm) regions. For the low albedo medium, the high absorp-

tion results in a very low radiance intensity in the large source-detector separations, and then the measurement of radiance field near the source is quite necessary.

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