Simple empirical master–slave dual-source configuration within the diffusion approximation enhances modeling of spatially resolved diffuse reflectance at short-path and with low scattering from a semi-infinite homogeneous medium

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Received 23 November 2016; revised 15 January 2017; accepted 15 January 2017; posted 17 January 2017 (Doc. ID 281482); published 8 February 2017

We present an empirical master–slave dual-source configuration within the diffusion approximation that enhances modeling of spatially resolved diffuse reflectance at short-path and with low scattering from a semi-infinite homogeneous medium when irradiated by a pencil beam. An isotropic virtual source positioned at a depth of $1/(\mu_s')$ is used as the master source. A second isotropic virtual source whose depth and intensity depend upon those of the master source and tissue property according to a set of simple empirical formulas is added as the slave source. When tested for a semi-infinite homogeneous medium, this master–slave dual-source model consistently produces the aggressive peaking of the diffuse reflectance toward the point of entry, which is significantly underestimated by the model prediction that involves only the master source. Monte Carlo simulations have shown the effectiveness of this empirical model at a short source–detector separation of $1/100$ of $1/(\mu_s')$ and an absorption to reduced scattering ratio as strong as 1, with an error within 20% in the near field ($1/10$ of $1/(\mu_s')$). © 2017 Optical Society of America

OCIS codes: (170.3660) Light propagation in tissues; (170.2150) Endoscopic imaging; (170.5280) Photon migration.

https://doi.org/10.1364/AO.56.001447

1. INTRODUCTION

Simple and transparent analytical approaches that adequately model spatially resolved diffuse reflectance at the quasi-diffusive regime, i.e., the source–detector separation (SDS) is 1 order less than the mean transport free path ($l'$), when irradiated by a pencil beam are of significant practical interest, regarding real-time forward computation for quantitative biopsy sensing [1] or depth-sampled endoscopic imaging [2]. While the radiative transport equation is accurate for all regimes of photon migration and any values of scattering albedo, it is sophisticated to implement [3,4] and is thus out of reach to most end users of forward computation. The standard diffusion approximation commonly treats the pencil beam irradiance as being from an isotropic virtual source located at a depth of $l'$ from the point of entry with the strength of the source often weighted by the scattering albedo and a factor associated with the transport scattering coefficient ($\mu_s' = 1/l'$), when only a homogeneous medium is concerned [5]. This single-source scheme within the diffusion approximation has for decades provided practically the simplest base for accurate modeling of the diffuse reflectance at the far field or the diffusive regime (i.e., $SDS \geq 10/l'$). However, at short SDS, as is needed for probing subsurface tissue properties through an endoscopic instrument channel [6] or laparoscopically using multiple fibers, the single-source diffusion approximation may significantly underestimate the aggressive peaking of the diffuse reflectance toward the point of entry, as is shown by numerous Monte Carlo (MC) [7–9] and experimental [10] studies. The single-source scheme within the diffusion approximation is also known to be less accurate when the absorption coefficient ($\mu_a$) of the medium increases to become comparable to the reduced scattering coefficient ($\mu_s'$), as is often the case at wavelengths that characterize chromophore absorption.

A rigorous reconfiguration of the photon diffusion analytics, by decomposing the phase-function dependency of scattering into an isotropic part and an anisotropic term, has provided...
by far the most accurate non-radiative-transfer-based modeling of the diffuse reflectance from a semi-infinite medium at a SDS as small as $l_s/100$, over a large range of anisotropy factor ($g = 0$ to 0.95), for typical turbid medium conditions, such as $\mu_s/\mu_t = 0.01$ [11]. This elegant model, which is in light of the delta-$P_1$ approximation [12, 13], is not completely transparent to all users, since it requires solving an integral equation of the phase-function-corrected photon fluence rate. A recent modification [14] to the standard diffusion approximation has employed multiple (two or more) virtual sources as the surrogate of the single source, leading to more accurate quantification of the diffuse reflectance at short-path from a low-albedo semi-infinite medium. The accuracy of this model increases with the number of virtual sources whose positions and intensities are determined by an optimization routine; thus, the implementation of it is less straightforward.

In this work, we present a simple, empirical modification within the diffusion approximation that is formulated transparently for effective modeling of diffuse reflectance at short-path from a semi-infinite medium when irradiated by a pencil beam. The central scheme of this model is a master–slave dual-source configuration. In other words, this model uses only two virtual sources, with one being the primary and the other being dependent upon the former one. The master source is an isotropic source to be placed at a depth of $1/\mu_s$, which is slightly different from the convention of a depth of $1/\mu_s$ in the standard diffusion approximation [15]. The slave source, which is also an isotropic one, is introduced to account for the aggressive peaking of the diffuse reflectance toward the point of entry, without distorting the spatially resolved patterns of diffuse reflectance at the far field. To facilitate this relatively localized effect on diffuse reflectance, the slave source must be placed much closer to the point of entry along the ballistic line of photon injection than does the master source. Intuitively, this slave source shall be placed at a depth associated with one scattering pathlength $1/\mu_s$, where $\mu_s$ is the scattering coefficient. The actual position of this slave source is set to be dependent upon the position of the master source and $g$. The relative intensity of this slave source with respect to the master source is set to depend upon $g$ and tissue attenuation. By having two isotropic sources whose positions and intensities are defined in closed form with transparency and only one open parameter, all salient conveniences associated with treating photon diffusion from an isotropic source are kept. In regard to the diffuse reflectance from a semi-infinite medium as applying to tissue probing, the convenience of this master–slave dual-source model is translated to simply applying the same boundary condition to the two sources. By making the second source slavery to the first source, this dual-source configuration is shown to robustly model the diffuse reflectance at short-path with SDS as small as 1/10 of $1/\mu_s$, and when the scattering albedo is low with the absorption coefficient $\mu_a$ reaching $\mu_s$, for scattering obeying the Henyey–Greenstein (HG) phase function.

2. METHODS AND MATERIALS

A. Empirical Model

The placement of the master–slave dual-source associated with a semi-infinite homogeneous medium when irradiated by a steady-state pencil beam and upon which the extrapolated boundary condition [15] is applied is illustrated in Fig. 1. The medium bounding with air is defined with the following optical properties: refractive index $n_{	ext{tiss}}$, $\mu_s$, $\mu_a$, $g$, $\mu_t = \mu_s(1 - g)$, diffusion coefficient $D = 1/(3(\mu_s + \mu_t))$, and effective attenuation coefficient $\mu_{\text{eff}} = \sqrt{\mu_a/D}$. The master source $S$ locates at a depth of $z_a = 1/\mu_s$, and has an intensity of $S = 1$ for a pencil beam incidence of unit intensity. We introduce a slave-source index $\eta(g, n)$ that is defined as

$$\eta(g, n) = [g \cdot \exp(1 - g)]^{1/n},$$

(1)

where $n$ is an open parameter that is demonstrated in the later section as affecting the model’s sensitivity to the scattering anisotropy $g$. With the slave-source index defined in Eq. (1), the depth of the slave source is set at

$$z_s = \frac{(1 - \eta)}{z_a},$$

(2)

and the intensity of the slave source $S^\ast$ is defined as the following:

$$S^\ast = S \cdot \exp \left[ -\mu_{\text{eff}} \frac{z_a + z_s}{2} \right] \cdot \eta,$$

(3)

The effect of the medium–air boundary is accounted for by introducing the extrapolated boundary [15] at which the composite photon fluence rate by the isotropic sources in the medium and their images w.r.t. the extrapolated boundary becomes zero. The extrapolated boundary is set at a distance of $z_b = 2AD$ away from the medium surface, where

![Fig. 1.](image_url) Positions of the master and slave sources are illustrated for a semi-infinite medium geometry. A pencil beam incident at the boundary is represented by the red arrowhead. The master source $S$ locates at a depth of $z_a = 1/\mu_s$ from the point of entry. The slave source $S^\ast$ locates at a depth of $z_s = 1/\mu_a$ that is more proximal to the point of entry than is the position of a depth of $1/\mu_s$. With respect to an extrapolated boundary that is placed $z_b$ away from the medium surface, the image source of $S$ is at $z_a + 2z_b$ away from the medium surface, and the image source of $S^\ast$ is at $z_s + 2z_b$ away from the medium surface.
The steady-state photon fluence rate at the detector as a result of the master source and its image w.r.t. the extrapolated boundary is

\[
\Psi_\text{real} = \frac{S}{4\pi D} \left[ \frac{\exp(-\mu_{\text{eff}} l_\text{real})}{l_\text{real}^3} - \frac{\exp(-\mu_{\text{eff}} l_\text{imag})}{l_\text{imag}^3} \right].
\]

(8)

The steady-state photon fluence rate at the detector as a result of the slave source and its image w.r.t. the extrapolated boundary is

\[
\Psi_\text{imag} = \frac{S^*}{4\pi D} \left[ \frac{\exp(-\mu_{\text{eff}}^* l_\text{real}^*)}{l_\text{real}^*^3} - \frac{\exp(-\mu_{\text{eff}}^* l_\text{imag}^*)}{l_\text{imag}^*^3} \right].
\]

(9)

The diffuse reflectance corresponding to photon measurement is the composition of both photon fluence rate and photon flux [13,16]. With the master–slave dual-source, the diffuse reflectance becomes

\[
R_{\text{Dual}}(\rho) = \frac{1}{\sqrt{2}} \left[ \frac{1}{4\pi} (\Psi(\rho) + \Psi^*(\rho)) + \frac{3}{4\pi} \left( J|_{\hat{z}^-}(\rho) + J^*|_{\hat{z}^-}(\rho) \right) \right].
\]

(13)

In comparison, the diffuse reflectance as a result of the single source follows the standard diffusion approximation as [13]

\[
R_{\text{Single}}(\rho) = 0.118 \Psi(\rho) + 0.306 J|_{\hat{z}^-}(\rho).
\]

(14)

B. MC Simulation

The spatially resolved diffuse reflectance associated with a semi-infinite medium under the irradiance of a pencil beam as modeled by Eq. (13) is compared against that by MC simulation and by Eq. (14). The MC simulation is performed using the “Monte Carlo Solver Panel” of Virtual Photonics General-Purpose ATK 2.2.0 Beta, by custom defining the positions of the detector in the user-editable Input File and changing the tissue optical properties using the online graphical user interface. A total of 1000 detector points were placed, corresponding to 3 decades of SDS of 0.01 ≤ \( \mu' \) ≤ 10. The simulations were executed with a total of 100,000 photons, for a tissue of 10 cm thickness and \( n = 1.40 \), with the HG phase function, as it is the one available on the MC solver.

3. RESULTS

The diffuse reflectance values modeled by Eqs. (13) and (14) for comparison with MC results are presented in this section. In all figures, the results by MC simulation are shown with discrete markers; the model predictions by Eq. (14) for the diffusion approximation involving one source are marked with dashed lines, and the mode predictions by the master–slave dual-source model of Eq. (13) are represented by solid lines.

A. Model Predictions of the Diffuse Reflectance from a Semi-Infinite Homogeneous Medium at the Same Scattering Properties but with Different Absorption Coefficients

Figure 2(a) presents the MC, dual-source, and single-source diffusion approximation modeling of diffuse reflectance over a SDS range of 0.01 ≤ \( \mu' \) ≤ 10 from a semi-infinite medium with \( \mu_s = 1 \text{ mm}^{-1} \), \( g = 0.9 \), and different \( \mu'_a \) values. The \( \mu_s \) values of 0.001, 0.01, 0.1, and 1 mm\(^{-1}\) correspond to \( \mu_s/\mu' \) of 0.001, 0.01, 0.1, and 1, respectively. The master–slave dual-source model predictions were implemented at \( n = 10 \). Figure 2(b) is Fig. 2(a) displayed with a logarithmic abscissa to magnify the short-path behaviors. The single-source model within the diffusion approximation starts to deviate from the MC results at a SDS of \( \mu' = [0.5, 1] \). In comparison, the master–slave dual-source model within the diffusion approximation duplicates the peaking of the diffuse reflectance toward the point of entry, which becomes increasingly aggressive as the SDS reduces from \( \mu'_s = 0.5 \) to \( \mu'_s = 0.01 \), with the values within 20% error comparing to MC results at SDS of
dual-source model predictions were implemented at μs‘ = 0.01 mm−1, 1 mm−1, and different values of scattering anisotropy of g = 0.5, 0.7, 0.8, 0.9, and 0.95. The diffuse reflectance curves are vertically shifted additional integer decades of magnitude in order to visualize the individual full-range patterns that are only slightly different at near field [13]. The master–slave dual-source model predictions were implemented at n = 10. Figure 4(b) is Fig. 4(a) displayed with a logarithmic abscissa, over a wider SDS range of 0.01 ≤ μs‘ ≤ 10 to magnify the short-path behaviors in the context of the entire 3-decade range of SDS. Additionally, the dual-source model outputs are plotted at different values of n = 1, 2, 4, and 10, to illustrate the near-field modulating effect of the slave-source index. It is found that, at smaller values of n (less than 4), this model could deliver more aggressive near-field peaking as the anisotropy factor reduces from g = 0.95 to 0.7, agreeing with the results of the more exact solution [11].

B. Model Predictions of the Diffuse Reflectance from a Semi-Infinite Homogeneous Medium at the Same Absorption and Reduced Scattering Coefficients but with Different Reduced Scattering Coefficients

Figure 3(a) presents the MC, dual-source, and single-source diffusion approximation modeling of diffuse reflectance over a SDS range of 0.01 ≤ μs‘ ≤ 10 from a semi-infinite medium with μs = 0.01 mm−1, μs = 10 mm−1, and different μs‘ values. The μs‘ values of 5, 2, 1, and 0.5 mm−1 correspond to g values of 0.5, 0.8, 0.9, and 0.95, respectively. The master–slave dual-source model predictions were implemented at n = 10. Figure 3(b) is Fig. 3(a) displayed with a logarithmic abscissa to magnify the short-path behaviors. The single-source model within the diffusion approximation starts to deviate from the MC results at a SDS of μs‘ ≈ [0.5, 1], depending upon the g values. In comparison, the dual-source model successfully duplicates the peaking of the diffuse reflectance over 0.01 ≤ μs‘ ≤ 1 for g values of 0.95, 0.9, and 0.8. At g = 0.5, the dual-source model is valid for a SDS of μs‘ ≥ 0.1.

C. Model Predictions of the Diffuse Reflectance from a Semi-Infinite Homogeneous Medium at the Same Absorption and Reduced Scattering Coefficients but with Different Scattering Coefficients

Figure 4(a) presents the dual-source and single-source diffusion approximation modeling of diffuse reflectance over a smaller SDS range of 0.01 ≤ μs‘ ≤ 1 from a semi-infinite medium with μa = 0.01 mm−1, μs‘ = 1 mm−1, and different values of scattering anisotropy of g = 0.5, 0.7, 0.8, 0.9, and 0.95. The diffuse reflectance curves are vertically shifted additional integer decades of magnitude in order to visualize the individual full-range patterns that are only slightly different at near field [13]. The master–slave dual-source model predictions were implemented at n = 10. Figure 4(b) is Fig. 4(a) displayed with a logarithmic abscissa, over a wider SDS range of 0.01 ≤ μs‘ ≤ 10 to magnify the short-path behaviors in the context of the entire 3-decade range of SDS. Additionally, the dual-source model outputs are plotted at different values of n = 1, 2, 4, and 10, to illustrate the near-field modulating effect of the slave-source index. It is found that, at smaller values of n (less than 4), this model could deliver more aggressive near-field peaking as the anisotropy factor reduces from g = 0.95 to 0.7, agreeing with the results of the more exact solution [11].

4. DISCUSSION

This empirical master–slave dual-source model contains one open parameter n that determines the depth and intensity of the slave source according to Eqs. (2) and (3). The effect of this open parameter on the depth and intensity of the slave source is illustrated in Fig. 5. Figure 5(a) evaluates the depth of the slave source zS w.r.t. the single-scatter length of 1/μs, as a function of g, at n values of 1, 2, 4, and 10. Figure 5(b) evaluates the strength of the slave source that depends upon g according to [g*exp(1 - g)]1/n, at the same set of n values of 1, 2, 4, and 10 as in Fig. 5(a). As is shown, higher g (or stronger scattering anisotropy) gives stronger slave source at a shallower relative depth (w.r.t. the mean free path). It is also shown that...
increasing \( n \) monotonically decreases the depth but increases the strength of the slave source.

This modulating effect of the open parameter \( n \) at near field has been indicated in Fig. 4. This near-field modulating effect of \( n \) also implies that by choosing different value of \( n \), it may be possible to adapt this empirical master–slave dual-source approach to modeling diffuse reflectance with scattering phase functions different from the HG function. Examining this hypothesis, however, would require access to MC solvers that can execute with different phase functions. Figure 4 has also shown that, as \( n \) exceeds 10, the diffuse reflectance at near the point of entry predicted by the dual-source model loses the sensitivity to \( g \), but becomes more accurate w.r.t. to the MC results for higher values of \( g \). Because biological tissues generally have a strong scattering anisotropy of \( g \geq 0.8 \), this dual-source model is thus expected to be useful for modeling diffuse reflectance from biological tissues, at a SDS of \( \rho\mu_t^0 \geq 0.1 \) as the region wherein the model estimation has consistently matched with MC results. Based on the testing of the model in this work on limited combinations of the medium properties associated with a homogeneous semi-infinite geometry, a value of \( n = 10 \) is recommended for use over the SDS that is not less than 1/10 of \( 1/\mu_t^0 \). For a soft tissue of a reduced scattering coefficient of 1 mm\(^{-1} \), it is expected that the model is useful over the SDS as small as 100 \( \mu \). This model, however, will need to be tested further with analytical extension to more realistic geometries, including layered media and media having localized absorbing or scattering heterogeneities.

The third curve in Fig. 3(b) when counted from the top, which corresponds to a set of medium properties of \( (\mu_s = 0.01 \text{ mm}^{-1}, \mu_t^0 = 1 \text{ mm}^{-1}, \text{ and } g = 0.9) \) is re-plotted in Fig. 6(a) to represent the ratio of the diffuse reflectance estimated by the dual-source (solid curve) over that by the MC, and the single-source (dashed curve) counterpart of the former. The ratio curves appear zigzagged as a result of the stochastic nature of the MC simulation. The zigzagging also increases at longer SDS as a result of the increased data variation at the longer SDS, wherein the MC engine produces a lesser number of countable photons. The two thin lines symmetric to and parallel with the thick horizontal line intersecting the ordinate at 1 represent the 20% error margin. The dual-source model performs consistently within 20% error over nearly the entire short-path region, even at SDS as small as \( \rho\mu_t^0 = 0.02 \), in comparison to the single-source model that starts to generate an error greater than 20% as \( \rho\mu_t^0 < 0.3 \) and increasing significantly as the SDS decreases. All curves of absolute comparisons demonstrated in this work show similar 20% error performances of the dual-source model prediction when converted to the ratios; therefore, only one representative ratio plot is presented in Fig. 6(a). For the specific set of model estimations shown in Fig. 6(a), the relative contribution of the slave source with respect to that of the master source to the diffuse reflectance is plotted in Fig. 6(b) over the same range of SDS as in Fig. 6(a). At far field, the contribution to the diffuse reflectance by the slave source is weaker than that by the master source, but not negligible (0.6807 of that of the master source at \( \rho\mu_t^0 = 10 \)). Conversely, in the near field, the contribution to the diffuse reflectance by the slave source increases dramatically as the SDS decreases, reaching 54.4260-fold of the master source at \( \rho\mu_t^0 = 0.01 \). It is the rapidly increasing contribution by the slave source toward the point of entry that has made the model prediction matching the MC results within 20% error over the near-field range.

It must be noted that this empirical model differs in several aspects from the conventional implementation of an isotropic source in the diffusion approximation that has accurately quantified the far-field diffuse reflectance: (1) the Fresnel reflection is not implemented, (2) the isotropic master source is placed at \( 1/\mu_t^0 \), not \( 1/\mu_t^0 \), (3) the strength of the master source is not weighted according to the scattering albedo, and (4) the strength of the master source is not modified due to tissue attenuation. Instead, this empirical model postulates the diffuse reflectance as originating from two sources, the master source with a constant “treatment” strength of \( S = 1 \), and the slave source with a “treatment” strength of \( S \leq 1 \) that is indeed dependent upon the scattering albedo and tissue attenuation. These “treatments” may seem to have caused the overall strength of the master–slave dual-source body to be greater than unity. However, this seemingly non-unity total strength of the master–slave dual-source body is actually compensated for in

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**Fig. 5.** (a) Depth of the slave source w.r.t. the single scatter path-length, as a function of \( g \), at different values of \( n = 1, 2, 4, \) and 10. The unit of the ordinate is thus \((1/\mu_s)\). (b) Relative intensity of the slave source w.r.t. the intensity \( S \), when excluding the exponential term in Eq. (3) at different values of \( n = 1, 2, 4, \) and 10.

**Fig. 6.** (a) Ratio of the diffuse reflectance estimated by the dual source (solid curve) over that by the MC, and the single-source (dashed curve) counterpart, for the third curve in Fig. 3(b) when counted from the top. (b) Relative contribution to the diffuse reflectance by the slave source over that of the master source.
Eq. (13) by a constant normalization factor 1/\sqrt{2} when referring to the formulations that approximate the diffuse reflectance or light intensity using both fluence rate and flux [13,16]. Interestingly, when the contribution to the diffuse reflectance by the slave source is identical to that by the master source (occurring around a S DS slightly smaller than 1/\mu_s' for the set shown in Fig. 6), Eq. (13) could simply approach

\[ R_{\text{Dual}}(\rho) = 0.113\Psi(\rho) + 0.338/|\langle z \rangle(\rho)|, \]

(15)

which is noticeably close to what is offered by the approximation given by Eq. (14) that fails to model the rapid peaking of the diffuse reflectance toward the point of entry. The normalization factor 1/\sqrt{2} can certainly bind directly to the master-source strength rather than appearing later in Eq. (13) at the computation of the diffuse reflectance, as is chosen now. Regardless of the step whereupon the factor of 1/\sqrt{2} actually weighs in, the ensemble of the empirical treatment as is culminated in Eq. (13) seems to be able to balance the contributions to the diffuse reflectance between the master source and the slave source to produce the pattern of rapidly peaking diffuse reflectance toward the point of entry that matches MC simulation consistently.

Quantitative optical imaging and sensing of highly scattering and anisotropic biological tissue by employing small source–detector separations are in need of rapid forward computation for real-time operation. However, a simple, transparent, and accurate analytical model of diffuse reflectance at short-path is not readily accessible to most investigators of photon propagation modeling. The master–slave dual-source approach demonstrated in this work, even though it is empirically formulated, is (1) simple to use following the common implementation of diffusion approximation with one isotropic source, (2) transparent, since all formulas are in closed explicit algebraic form, with only one open parameter to be determined w.r.t. the recommended value, (3) accurate for a medium of high anisotropy and a source–detector separation greater than 1/10 of 1/(reduced scattering coefficient), and (4) effective for a high absorption medium with the absorption as strong as the reduced scattering. The empiricism of this model, however, does indicate potential for future improvement when the merit of the master–slave dual-source scheme is continued. Future works that this master–slave dual-source model could extend to include rapid forward modeling associated with layered media, media with single heterogeneity, media with non-planar boundaries, frequency-domain and time-domain measurements, fluorescence measurement, and single-fiber detection.

5. CONCLUSIONS

In conclusion, we have demonstrated a simple empirical master–slave dual-source configuration within the diffusion approximation that enhances modeling of spatially resolved diffuse reflectance at short-path and with low scattering from a semi-infinite homogeneous medium when irradiated by a pencil beam. The commonly used isotropic virtual source positioned near a depth of 1/\mu_s' is used as the master source. A second isotropic virtual source whose depth and intensity depend upon those of the master source and tissue property according to simple empirical formulas is added as the slave source. When compared to the standard diffusion approximation involving only the master source, this master–slave dual-source model consistently produces the aggressive peaking of the diffuse reflectance toward the point of entry for a semi-infinite homogeneous medium. MC simulations have shown the effectiveness of this model at a source–detector distance as small as 1/10 of 1/\mu_s' and a reduced scattering-to-absorption ratio as low as 1, with an error of 20% in the near field of \rho \mu_s' \geq 0.1.

Funding. Technology Business Development Program of Oklahoma State University (OSU).

Acknowledgment. This work was made possible by using Virtual Photonics, which was developed by the Laser Microbeam and Medical Program (LAMMP; P41 EB015890-33), an NIH/NIBIB Biotechnology Resource Center.

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