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Effect of Spatially Distributed Light Sources on the Frequency-Domain Solution to the Diffusion Equation

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ABSTRACT

We have investigated the accuracy of the frequency-domain, diffusion equation Green's function in modeling optical signals in turbid media. Our optical measurements were conducted in strongly scattering media having absorption coefficients in the range 0.035-0.14 cm⁻¹ and reduced scattering coefficients in the range 5-22 cm⁻¹. The optical signal was both delivered to and collected from the sample by means of optical fibers. We have verified that the r -independent factor in the Green's function does not agree with the experimental data. This discrepancy shows that the photons launched in the medium by an optical fiber cannot be modeled by a point source located at a fixed position. These results have no influence on multi-distance measurement protocols (which only employ the r -dependent part of the solution), while they must be considered when calibration measurements on a known sample are performed.

Keywords: diffusion equation, Green's function, frequency-domain, strongly scattering media

1. INTRODUCTION

The diffusion equation is widely used to describe the propagation of light in strongly scattering media. In near-infrared (NIR) spectroscopy of biological tissues (which act as strongly scattering media), the interrogating light beam is usually delivered by an optical fiber. In the assumption that the effective photon source is point-like, the diffusion equation Green's function provides the solution for the distribution of the optical energy density in the tissue. The frequency-domain Green's function for infinite media is the following:¹⁻³

$$G(r, \omega) = \frac{1}{4\pi\nu D} \frac{e^{-kr}}{r}, \quad (1)$$

where r is the distance from the source, ω is the angular modulation frequency, ν is the speed of light in the medium, D is the diffusion coefficient ($D=1/3\mu_s'$ with μ_s' reduced scattering coefficient), and k is a complex wave vector given by $[(\nu\mu_a - i\omega)/(\nu D)]^{1/2}$, with μ_a absorption coefficient. It has been demonstrated that the r -dependence predicted by Eq. (1) accurately models the experimental data at sufficiently large distances from the source.⁴ This fact has led to the development of a multi-distance measurement protocol for the quantitative spectroscopy of uniform, strongly scattering media.⁴ In the presence of macroscopic inhomogeneities (such as bones or large blood vessels) the multi-distance method may not be as effective as it is in uniform media. Alternative approaches employing one fixed source-detector separation have been proposed.⁵ One of those approaches is based on a preliminary calibration measurement on a medium with known optical properties.^{6,7} This latter approach is not just based on the r -dependence of Eq. (1) but also on the pre-exponential factor $(4\pi\nu D)^{-1}$. This paper shows that such a pre-exponential factor does not correctly model the experimental data. The reason for this failure is that the effective photon source cannot be simply described by a point source located in a fixed position and having a fixed strength.

2. THEORY

The frequency-domain Green's function given in Eq. (1) describes the photon density generated in a uniform, infinite, turbid medium, by a unit-power, point-like photon source located at the origin and emitting at angular frequency ω . In the presence

of a spatially extended photon source described by $q(\mathbf{r}, \omega)$ (source power per unit volume), the solution for the photon density $U(\mathbf{r}, \omega)$ is given by the spatial convolution:

$$U(\mathbf{r}, \omega) = q(\mathbf{r}, \omega) * G(\mathbf{r}, \omega) = \iiint q(\mathbf{r}', \omega) G(|\mathbf{r} - \mathbf{r}'|, \omega) d^3 \mathbf{r}' \quad (2)$$

For a spherically symmetric photon source $q(r, \omega)$, the convolution integral becomes:

$$U(r, \omega) = \frac{1}{2vDr} \int_0^\infty r' q(r', \omega) \frac{e^{-k(r+r')} - e^{-k|r-r'|}}{-k} dr' = \frac{1}{2vDr} \left[\frac{e^{-kr}}{-k} \int_0^\infty e^{-kr'} r' q(r', \omega) dr' - \frac{e^{-kr}}{-k} \int_0^r e^{kr'} r' q(r', \omega) dr' - \frac{e^{kr}}{-k} \int_r^\infty e^{-kr'} r' q(r', \omega) dr' \right] \quad (3)$$

If $q(r, \omega)$ is 0 at $r > r_0$, the solution for $r > r_0$ simplifies to:

$$U(r > r_0, \omega) = \frac{1}{vDk} \left[\int_0^{r_0} r' q(r', \omega) \sinh(kr') dr' \right] \frac{e^{-kr}}{r} \quad (4)$$

Equation (4) points out two important facts:

- (i) In the case of a spherically symmetric photon source which is confined within the region $r < r_0$, the r -dependence of the photon density at $r > r_0$ is the same as that of the Green's function, namely $\exp(-kr)/r$;
- (ii) The pre-exponential factor of $U(r > r_0, \omega)$ is significantly different than that of the Green's function, it is complex, and it contains the absorption coefficient (in k) which does not appear in the Green's function pre-exponential factor.

The first point (i) states that a multi-distance measurement is not affected by changes in the spatial extent of a spherically symmetric photon source, provided that the measurements are conducted out of the source. The second point (ii) shows that the pre-exponential factor is sensitive to the details of the photon source spatial distribution.

To model the anisotropic light emission of an optical fiber, we have considered a hemispheric, uniform photon source centered at the fiber tip and having a radius γ . In spherical coordinates (with the polar axis along the fiber), the source term $q(r', \theta', \phi', \omega)$ is written as:

$$q(r', \theta', \phi', \omega) = \begin{cases} \frac{3S_{\text{eff}}(\omega)}{2\pi\gamma^3} & \text{for } 0 \leq r' \leq \gamma \text{ and } 0 \leq \theta' \leq \frac{\pi}{2} \\ 0 & \text{for } r' > \gamma \text{ or } \frac{\pi}{2} < \theta' \leq \pi \end{cases} \quad (5)$$

where S_{eff} is the effective source power. The results for the photon density U_{hs} determined by this source term can be calculated by carrying out the convolution integral of Eq. (2). The result at distances such that $r^2 \gg \gamma^2$ and at $\theta = 0$ (i.e. in the direction of the optical fiber) is the following:

$$U_{\text{hs}}(r, \theta = 0, \omega) \Big|_{r^2 \gg \gamma^2} = S_{\text{eff}}(\omega) \frac{3[1 + (k\gamma - 1)e^{k\gamma}]}{k^3 \gamma^3} \frac{1}{4\pi vD} \frac{e^{-kr}}{r} \quad (6)$$

Once again, the r -dependence is the same as that of the Green's function, while the pre-exponential factor is different. The experimentally measured quantity is the radiance integrated over the acceptance angle of the optical fiber used to collect the light. In the diffusion approximation, the radiance along direction $\hat{\Omega}$ is given by:

$$\text{Radiance} = \frac{vU}{4\pi} - \frac{3vD}{4\pi} \nabla U \cdot \hat{\Omega} \quad (7)$$

The theoretical prediction for the detected signal is the integral of Eq. (7) over the acceptance angle of the detection fiber. For the case of a photon density $U(r, \omega) \propto \exp(-kr)/r$, and for a detector optical fiber pointing toward the source, the integral of Eq. (7) yields the following expression for the detected photon current I :

$$I = \Delta A \frac{\nu U(r, \omega)}{2} \left[\frac{1}{4} (1 - \cos 2\theta_f) + D \frac{1+kr}{r} (1 - \cos^3 \theta_f) \right], \quad (8)$$

where ΔA is the cross section of the fiber core, and θ_f is the acceptance angle of the optical fiber.

3. MATERIALS AND METHODS

The strongly scattering medium is a 9-liter aqueous suspension of Liposyn and black India ink. The Liposyn concentration is varied to obtain reduced scattering coefficients in the range $5\text{--}22\text{ cm}^{-1}$ (with constant $\mu_a = 0.035\text{ cm}^{-1}$). The black India ink concentration is varied to obtain absorption coefficients in the range $0.035\text{--}0.14\text{ cm}^{-1}$ (with constant $\mu_s' = 16\text{ cm}^{-1}$). The light source is a 780 nm laser diode (Sharp LT023), whose intensity is modulated at 120 MHz by a radio frequency synthesizer (Marconi 2022A). The average optical power is about 3 mW and the modulation depth is nearly 100%. The laser diode is coupled to a 2 mm optical fiber with a numerical aperture of 0.5. The optical signal is collected by an optical fiber (2 mm core diameter, 0.5 numerical aperture) which delivers the signal to a photomultiplier tube (PMT) (Hamamatsu R928). The radio frequency signal (120 MHz) is down converted to 400 Hz by heterodyning methods and is processed to yield an average value (dc), amplitude (ac), and phase (Φ) of the detected photon density wave.⁸ The two optical fibers face each other and they are deeply immersed in the sample so that an infinite geometry can be assumed. The detector fiber is moved by a step motor to perform measurements at different source-detector distances. The range of distances considered in this work is 0-2 cm. The measurements over the wide intensity dynamic range ($\sim 10^5$) required for this range of distances was achieved by inserting appropriate neutral density filters in front of the PMT. The high power supply of the PMT was never changed during the experiment. A schematic diagram of the experimental setup is shown in Fig. 1.

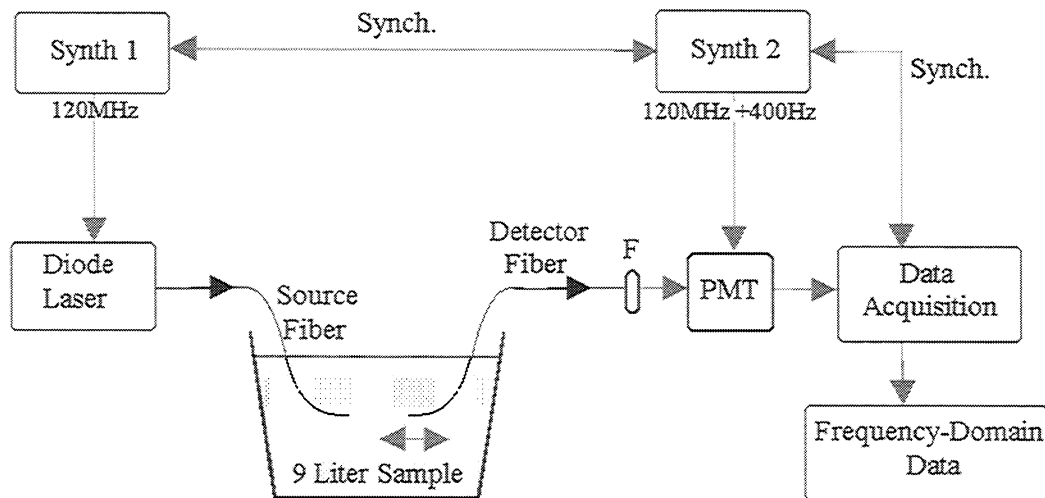


Fig. 1. Experimental setup. A radio frequency synthesizer (Synth 1) modulates the intensity of the diode laser at 120 MHz, while synthesizer 2 modulates the gain of the photomultiplier tube (PMT) detector at 120 MHz + 400 Hz. The light collected by the detector fiber is attenuated by a neutral density filter (F). The PMT output is processed to yield the frequency-domain parameters (dc intensity, ac amplitude, and phase).

4. RESULTS

In the frequency-domain, the detected signal can be written as $I(r,\omega)\exp[i\Phi(r,\omega)]$, where $I(r,\omega)$ is the amplitude and $\Phi(r,\omega)$ is the phase of the intensity at distance r and angular frequency ω . At distances from the source much greater than $1/\text{Re}[k]$, the two functions $\ln[rI(r,\omega)]$ and $\Phi(r,\omega)$ depend linearly on r . The pre-exponential factor (which can in principle be complex) in the expression for the photon density affects the intercept of these straight lines, but not the slopes. For this reason, we have investigated the intercepts which we obtained experimentally by extrapolating to $r = 0$ the straight lines measured at distances greater than $1/\text{Re}[k]$. The results are shown in Figs. 2 and 3.

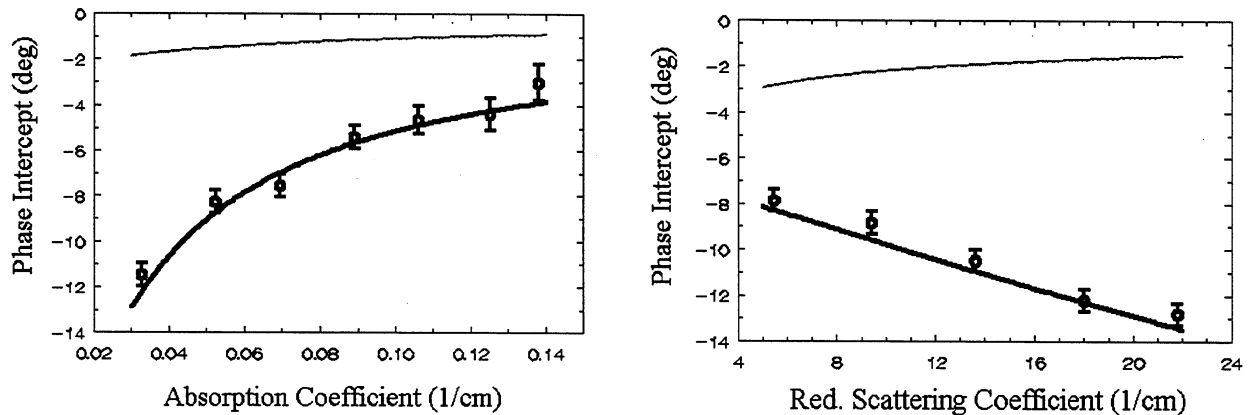


Fig. 2. Phase intercept (i.e. extrapolated value at $r = 0$ of the straight line given by the phase as a function of r) versus μ_a (panel (a)), and versus μ_s' (panel (b)). In (a), μ_s' is 16 cm^{-1} , whereas in (b), μ_a is 0.035 cm^{-1} . The symbols are the experimental values obtained from the phase data measured at r ranging from 1.5 to 2 cm. The lines are the phase intercepts predicted by diffusion theory for a point source (thin lines) and for the effective hemispheric source (thick lines).

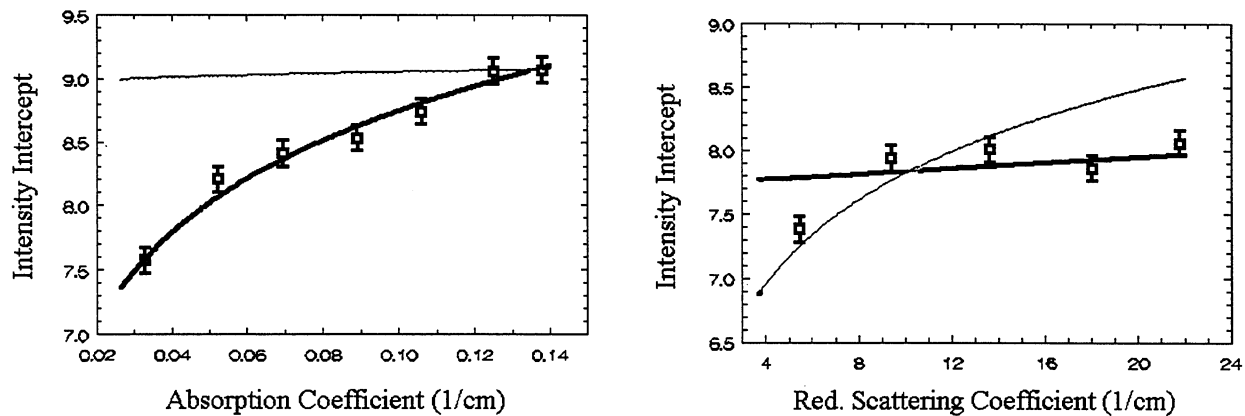


Fig. 3. Intensity intercept (i.e. extrapolated value at $r = 0$ of the straight line given by the $\ln[rI(r,0)]$ as a function of r) versus μ_a (panel (a)), and versus μ_s' (panel (b)). In (a), μ_s' is 16 cm^{-1} , whereas in (b), μ_a is 0.035 cm^{-1} . The symbols are the experimental values obtained from the intensity data measured at r ranging from 1.5 to 2 cm. The lines are the intensity intercepts predicted by diffusion theory for a point source (thin lines) and for the effective hemispheric source (thick lines).

The symbols represent the experimentally determined intercepts, the thin lines are obtained from the Green's function (Eq. (1) into Eq. (7)), and the thick lines are obtained from the hemispheric effective source term (Eq. (6) into Eq. (7)).

Equation (6) contains two parameters (γ and S_{eff}) that need to be determined. Since S_{eff} (being real) does not affect the phase intercept, we have initially obtained an expression for γ that is consistent with the experimental phase intercepts:

$$\gamma = \frac{1}{\text{Re}\left[k(\mu_a, \mu_{s0}', \omega)\right]}, \quad (9)$$

where $\mu_{s0}' = 16 \text{ cm}^{-1}$. We thus have an effective source whose radius depends on μ_a , ω , but (surprisingly) not on μ_s' . The second parameter, S_{eff} , has been empirically determined to best reproduce the intensity intercepts:

$$S_{\text{eff}} \propto S \frac{\mu_a}{\mu_s'}, \quad (10)$$

where S is the actual source power, i.e. the number of photons per second emitted by the tip of the source fiber.

The absolute values of the intercepts are meaningful only in the phase graphs (Fig. 2) (where the phase reference, set to zero, is taken at $r = 0$, i.e. when the source and detector fibers are in contact), and not in the intensity graphs (Fig. 3) where the unknown instrumental response cannot be accounted for. Consequently, the lines in Fig. 2 are plotted as they are obtained from the calculations, while the lines in Fig. 3 are shifted by an arbitrary offset.

5. DISCUSSION AND CONCLUSION

By considering an effective hemispheric photon source centered at the tip of the source fiber, we have been able to derive a pre-exponential factor (in the expression for the photon density) that models the experimental results much better than the pre-exponential factor in the Green's function. The two parameters that describe the hemispheric photon source, namely the radius γ and the effective source power S_{eff} , depend on the optical coefficients and are given in Section 4. In our experimental conditions, the values of γ range from 0.4 to 0.8 cm. These values are on the order of the diffusion length (not the mean free path) in the medium. The effective source power S_{eff} is proportional to the ratio μ_a/μ_s' . The increase of S_{eff} with μ_a seems paradoxical but it is explained by the fact that the volume of the effective source decreases as $\mu_a^{-3/2}$, so that the probability of photon absorption within the effective source volume is decreased.

In conclusion, we have shown that the r -dependence of the optical signal collected in strongly scattering media is well described by the Green's function, even if the effective photon source is spatially distributed (and spherically symmetric). By contrast, the pre-exponential factor is significantly affected by the details of the spatial distribution of the effective source. We have considered a hemispheric photon source of radius γ centered at the tip of the source fiber. The experimental results over a wide range of optical coefficients (0.035 - 0.14 cm^{-1} for μ_a , 5 - 22 cm^{-1} for μ_s') could be reproduced by letting both the size and the power of the effective photon source be a function of the optical properties of the medium.

6. ACKNOWLEDGMENTS

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