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Diffusion theory for multi-layered scattering media

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ABSTRACT

We present an approximation to light propagation through skin using an improved multilayered diffusion equation. This equation allows for the influence of multiple layers on diffusely reflected light to be considered; which is accomplished by embedding imaginary point sources in the medium that correspond to each layer's transport mean free path. The new approximation is then compared to a previous two-layer solution by Farrell et al. to verify improvement as well as to results from Monte Carlo simulations to verify accuracy.

Keywords: tissue, Optical diagnostics for medicine, Medical optics and biotechnology, Spectroscopy, Diffusion

1. INTRODUCTION

There is great interest in determining the optical parameters of biological tissue non-invasively for a wide range of applications in therapeutics and diagnostics. The first step in this process is to develop an accurate and relatively fast method that can be used to simulate the propagation of light through tissue. This is hampered by the difficulty that light is highly scattered by most tissue. This means that the optical signal undergoes a large number of scattering events before its photons exit the medium. A signal that contains photons with no correlation between their entering and exiting directions are likely to have gone through large distances in the tissue. While these photons carry information about the medium, their chaotic paths are difficult to resolve. The challenge is in developing a forward method to approximate the signal inside the tissue.

One technique for finding the diffuse reflectance from highly scattering tissue is to use the homogenous diffusion approximation to the Radiative Transport Equation. This method assumes that the light reflected from tissue due to an incident collimated beam can be modeled as light coming from an equivalent isotropic point source located within a homogenous medium. For this to work, the tissue's reduced scattering (μ_s') is assumed to be much higher than the absorption coefficient (μ_a). The reduced scattering coefficient is arrived at by

$$\mu_s^{'} = \mu_s(1-g) \qquad (1)$$

where μ_s and g are the scattering and anisotropy coefficients respectively. The isotropic point source is located at one transport mean free path inside the medium ($1/\mu_t$'), where

$$\mu_t^{'} = \mu_s^{'} + \mu_a \qquad (2)$$

Detailed discussions of this method for normal incidence can be found in Farrell et al.[1] and Oblique incidence in Wang et al. [2]

As mentioned above these two methods model tissue as a homogenous medium. For skin and other complicated tissues this is not an accurate assumption. At a minimum skin contains both the epidermis and dermis layers. If these are optically thin we also have to take into account how the subcutaneous tissue influences the light signal. To improve upon this assumption Kienle et al.[3] have developed a two-layer

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solution to the diffusion equation that models the light reflected from skin as coming from a single equivalent point source. The solution assumes that the first layer is optically thick and the isotropic point source is located at one transport mean free path within it. This solution does not fully incorporate the effects of the second layer; which is a problem if the first is optically thin. We present here a solution to the diffusion equation that utilizes an equivalent point source for each of the two layers; which allows us to overcome these difficulties.

2. METHODOLOGY

2.1. Theory

The problem of interest has an infinitesimal, collimated beam incident at a normal angle onto scattering medium made up of two homogenous layers. The coordinate system is set up so that its origin is located at the point where the beam enters the medium with its z+ axis is pointing down. The first layer has a

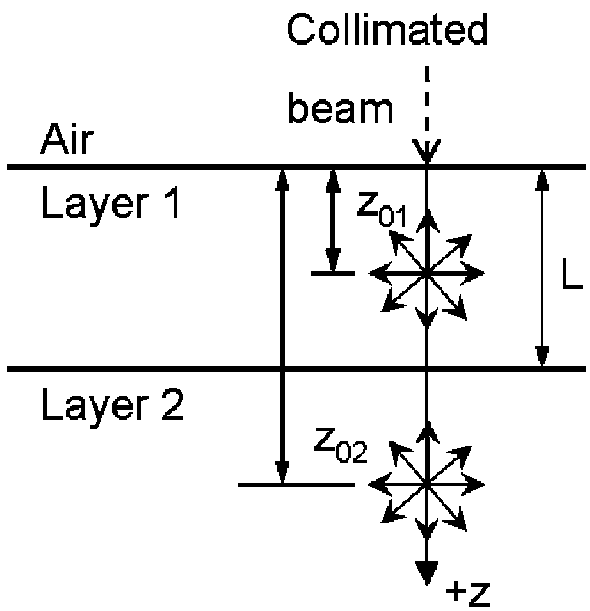

Figure 1: Geometry of two-layer solution to the diffusion equation. The positions of the equivalent isotropic point sources are denoted by z_{01} and z_{02}. L is the thickness of layer 1 and the positive z direction is into the tissue.

thickness of L and the second layer extends to infinity. Both layers are considered to be radially homogenous. The resulting fluence rate (Φ) and reflectance is modeled by replacing the incident collimated beam with an equivalent isotropic point source in each layer. The geometry of this problem is shown in Figure 1. The optical properties for layers one and two are denoted by their subscripts.

The locations of the point sources (z_{0i} for i=1,2) are given by the mean intensity over the total intensity of light's fluence within each layer.

$$
z_{01} = \frac{\int_0^L z \exp(-\mu_{t1}^{'} L) dz}{\int_0^L \exp(-\mu_{t1}^{'} L) dz} = \frac{1-(\mu_{t1}^{'} L + 1)\exp(-\mu_{t1}^{'} L)}{\mu_{t1}^{'}(1-\exp(-\mu_{t1}^{'} L))}
$$

$$
z_{02} = \frac{\int_L^\infty z \exp(-\mu_{t1}^{'} L - \mu_{t2}^{'}(z-L)) dz}{\int_L^\infty \exp(-\mu_{t1}^{'} L - \mu_{t2}^{'}(z-L)) dz} = L + \frac{1}{\mu_{t2}^{'}} \qquad (3)
$$

where L is the thickness of the first layer. The corresponding source strengths (or weightings) for these positions are

$$
S_{w1}(z) = \int_0^L a_1^{'} \mu_{t1}^{'} \exp(-\mu_{t1}^{'} z) dz = a_1^{'}(1-\exp(-\mu_{t1}^{'} L))
$$

$$
S_{w2}(z) = \int_L^\infty a_2^{'} \mu_{t2}^{'} \exp(-\mu_{t2}^{'}(z-L) - \mu_{t1}^{'} L) dz = a_2^{'} \exp(-\mu_{t1}^{'} L) \qquad (4)
$$

where a_i' is the transport albedo for each layer: $a_i' = \mu_{si}'/\mu_{ti}'$, i=1 and 2. We can see that if the first layer becomes too thick, S_{w2} approaches zeros and z_{01} approaches $1/\mu_{t1}'$. This then becomes the single-layer diffusion equation.

The steady-state diffusion equation becomes

$$
D_1 \nabla^2 \Phi_1(r) - \mu_{a1} \Phi_1(r) = -S_{w1} \delta(x, y, z - z_{01})
$$

$$
D_2 \nabla^2 \Phi_2(r) - \mu_{a2} \Phi_2(r) = -S_{w2} \delta(x, y, z - z_{02}) \qquad (5)
$$

where $D_i = \dfrac{1}{3(\mu_{ai} + \mu_{si}^{'})}$ is the diffusion constant and $r=(x,y,z)$. The dirac delta functions correspond to each source position.

These equations can be solved for by first taking their two-dimensional Fourier transform:

$$
\frac{\partial^2}{\partial z^2} \phi_i(z, s_a, s_b) - \alpha_i^2 \phi_i(z, s_a, s_b) = -\frac{S_{wi}}{D_i} \delta(z - z_{0i}) \qquad i=1,2 \qquad (6)
$$

where s_a and s_b are spatial frequency dummy variables. We can take advantage of the radial homogeneity by saying that $s_i^2 = s_{ai}^2 + s_{bi}^2$ and by introducing the variable $\alpha_i^2 = \dfrac{D_i s_i^2 + \mu_{ai}}{D_i}$.

Using a Green's function and the following boundary conditions can solve for equation 4:
First, we use the extrapolated boundary condition for a matched index of refraction at the tissue-air interface to give us

$$\phi_1(-z_b, s) = 0 \tag{7}$$

where

$$z_b = 2AD_1 \tag{8}$$

is the position of the extrapolated boundary. The negative sign implies the boundary is located above the medium. The boundary condition is handled in the term A

$$A = \frac{1 + r_{eff}}{1 - r_{eff}} \tag{9}$$

where r_{eff} is the number of photons internally, diffusely reflected at the boundary. For an index-matched boundary, r_{eff} is zero and A=1. Haskell et al.[4] discusses how to find r_{eff} for index mismatches at the boundary.

Using the supposition that the second layer is infinite we get

$$\phi_2(\infty, s) = 0 \tag{10}$$

If we assume tissue layers have similar indices of refraction, we get

$$\frac{\phi_1(L,s)}{\phi_2(L,s)} = \frac{n_1^2}{n_2^2} = 1 \tag{11}$$

$$D_1 \left.\frac{\partial \phi_1(z,s)}{\partial z}\right|_{z=L} = D_2 \left.\frac{\partial \phi_2(z,s)}{\partial z}\right|_{z=L} \tag{12}$$

We then get the solution to equation 4 to be

$$\phi_1(z,s) = \frac{\exp(-\alpha_1(z_b+z))\left(S_{w1}\left(\cosh(\alpha_1(L-z_{01})) - \frac{\alpha_2 D_2}{\alpha_1 D_1}\sinh(\alpha_1(L-z_{01}))\right) - S_{w2}\exp(-\alpha_2(z_{02}-L))\right)}{2\left(\alpha_2 D_2 \sinh(\alpha_1(z_b+L)) + \alpha_1 D_1 \cosh(\alpha_1(z_b+L))\right)}$$
$$+ \frac{\left(\exp(-\alpha_1 L) S_{w1}\left(1 - \frac{\alpha_2 D_2}{\alpha_1 D_1}\right)\sinh(\alpha_1(z_b+z_{01})) + S_{w2}\exp(-\alpha_2(z_{02}-L) + \alpha_1 z_b)\right)\exp(\alpha_1 z)}{2\left(\alpha_2 D_2 \sinh(\alpha_1(z_b+L)) + \alpha_1 D_1 \cosh(\alpha_1(z_b+L))\right)} + \frac{S_{w1}\exp(-\alpha_1 |z-z_{01}|)}{2 D_1 \alpha_1} \tag{13}$$

for 0<z<L and

$$\phi_2(z,s) = \frac{-S_{w1}\exp\left(-\alpha_1(z_b+z_{01})-\alpha_2 z\right)}{2\exp(-\alpha_2 L)\left(\alpha_2 D_2 \sinh(\alpha_1(z_b+L))+\alpha_1 D_1\cosh(\alpha_1(z_b+L))\right)}$$
$$-\frac{\cosh\left(\alpha_1(L+z_b)\right)\exp(-\alpha_2 z)\left(\frac{\alpha_1 D_1}{\alpha_2 D_2}S_{w2}\exp\left(-\alpha_2(z_{02}-L)\right)-S_{w1}\exp\left(-\alpha_1(L-z_{01})\right)\right)}{2\exp(-\alpha_2 L)\left(\alpha_2 D_2 \sinh(\alpha_1(z_b+L))+\alpha_1 D_1\cosh(\alpha_1(z_b+L))\right)}$$
$$-\frac{\sinh\left(\alpha_1(L+z_b)\right)\exp(-\alpha_2 z)\left(S_{w2}\exp\left(-\alpha_2(z_{02}-L)\right)+S_{w1}\exp\left(-\alpha_1(L-z_{01})\right)\right)}{2\exp(-\alpha_2 L)\left(\alpha_2 D_2 \sinh(\alpha_1(z_b+L))+\alpha_1 D_1\cosh(\alpha_1(z_b+L))\right)}$$
$$+\frac{S_{w2}\exp\left(-\alpha_2\left|z-z_{01}\right|\right)}{2\alpha_2 D_2} \tag{14}$$

for z > L.

We then need to take the inverse Fourier transform to convert equations 13 and 14 into their final solutions.

$$\Phi_i(x,y,z) = \frac{1}{4\pi^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\phi_i(z,s)\exp(-i(s_1 x+s_2 y))ds_1 ds_2 \tag{15}$$

To simplify equation 15 we can take advantage of the radial homogeneity of the model and convert to cylindrical coordinates.

$$\Phi_i(\rho,z) = \frac{1}{2\pi}\int_0^{\infty} s\phi_i(z,s)J_0(s\rho)ds \tag{16}$$

where J_0 is a zeroth order Bessel function of the first kind. These equations cannot be solved in closed form, so we employ the Simpson's quadrature[5] to find the numerical solution. It is not necessary to integrate to infinity and infact, we must impose a limiting condition due to the hyperbolic functions or else computer round off error could drastically influence the final answer. For this situation, it can be assumed that the function ϕ_i is monotonically decreasing as z grows. If ϕ_i changes direction and begins to grow, we know that the error is influencing the results and should end our integration.

For an index-matched boundary, the spatially resolved reflectance is given from the fluence as[6]

$$R(\rho) = \frac{1}{4}\Phi_1(\rho,z=0)+\frac{1}{2}D_1\left.\frac{\partial\Phi_1(\rho,z)}{\partial z}\right|_{z=0} \tag{17}$$

this equation can be simplified by using[4]

$$\Phi_1(\rho,z=0) = A\left.\frac{\partial\Phi_1}{\partial z}\right|_{z=0} \tag{18}$$

Substituting equation 18 into 17 and using A=1 from above, we get

$$R(\rho) = \frac{1}{2}\Phi_1(\rho, z = 0) \tag{19}$$

This discussion has been limited to a two-layer tissue structure but can be extended to any number of layers. First place an equivalent isotropic point source in each layer using equations 3 and 4 for the locations and weightings. Then use equations 11 and 12 to find the boundary conditions at the borders of each layer and then solve for the constants of integration.

2.2. Simulations

For the purposes of this paper the Monte Carlo simulation shall be the "gold standard." A detailed discussion can be found in Wang et all[7] but for our purposes it will suffice to say that Monte Carlo uses a weighted random walk to predict the paths of individual photons through a turbid medium. Since the simulation is statistical in nature, it requires a large number of photons to be run so that the results are within acceptable error bounds. The two-source solution presented within this paper and the single-source solution mentioned above[3] were then programmed so that we could verify the improved accuracy of our method.

Two Monte Carlo simulations were run to test the approximations using the parameters listed in Figure 2. The optical parameters were kept the same for each simulation with only the depth changing. This is to test the validity of each approximation for an optically thick and thin first layer. Optically thick is defined as $L>1/\mu_{t1}'$.

	Run 1	**Run 2**
μ_{s1}' (cm-1)	10	10
μ_{s2} (cm-1)	12	12
μ_{a1} (cm-1)	.2	.2
μ_{a2} (cm-1)	.01	.01
L (cm)	.12	.05

Figure 2: Optical Parameters for simulations

3. RESULTS

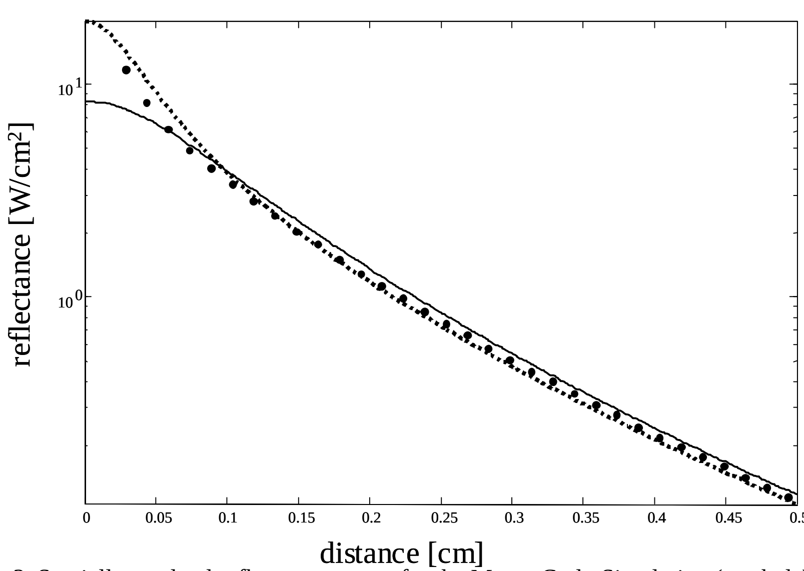

Figure 3: Spatially resolved reflectance curves for the Monte Carlo Simulation (symbols), and the single (solid) and double source (dotted) approximations.

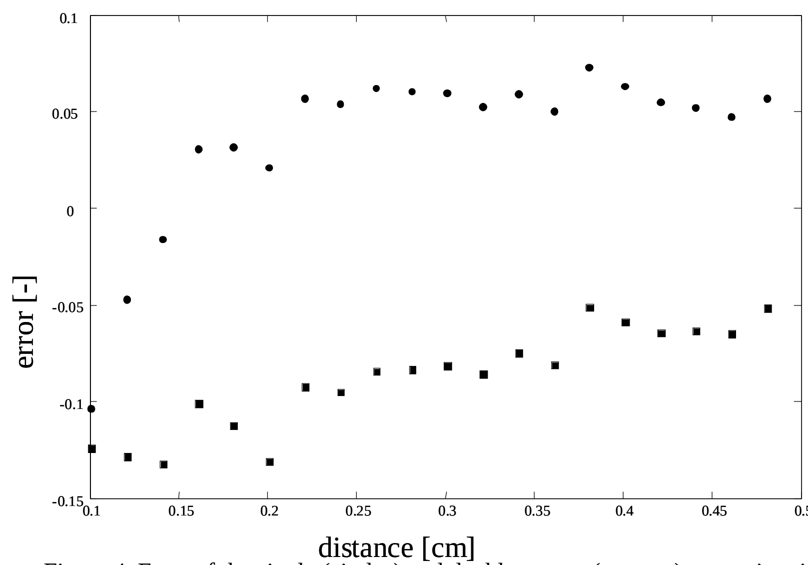

Figure 4: Error of the single (circles) and double-source (squares) approximations versus Monte Carlo results

The results for the reflectance due to the parameters listed under run 1 are shown in Figure 3. The reflectance from the two-source approximation seems to agree with the Monte Carlo results at a distance of 0.1 cm from the source. We can see from figure 4 that the two-source approximation's error does not exceed 7%. We can see that the single source approximation has a maximum error of about 10% in the same area.

We can see that the reflectance due to the two-source diffusion approximation becomes accurate much earlier - at a distance of less than 0.05 cm. It is not generally true that the two-source approximation is accurate closer to the source than the single source approximation.

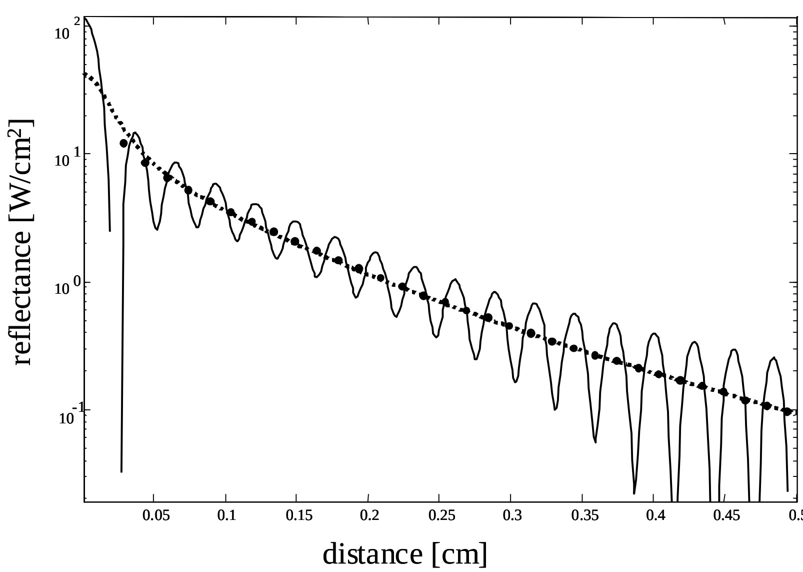

Figure 5: Spatially resolved reflectance curves for the Monte Carlo Simulation (symbols), and the single (solid) and double source (dotted) approximations

The results for an optically thin layer (Figure 2, run 2) are shown in Figure 5. We see that the reflectance calculated from the single-source approximation oscillates wildly as compared to the Monte Carlo results. The error is above 100% at the local maxima's and minima's of the single-source reflectance curve.

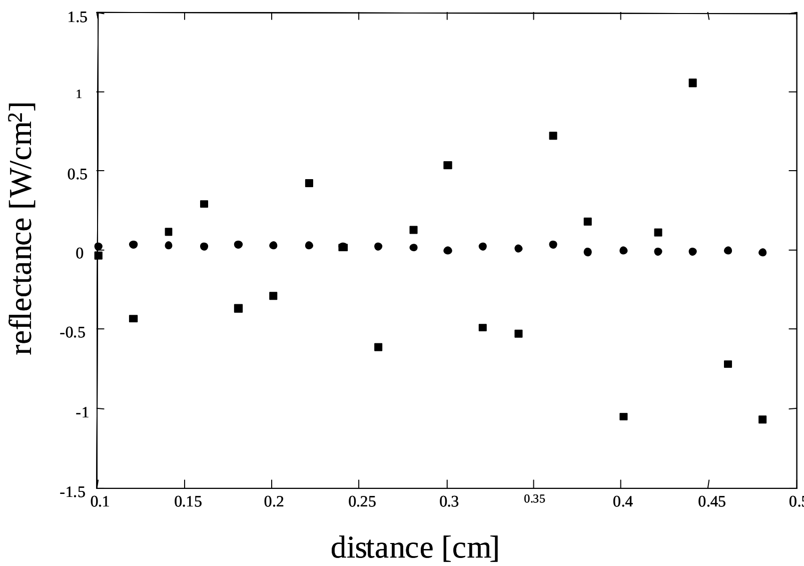

Figure 6: Error of the single (circles) and double-source (squares) approximations versus Monte Carlo results

Clearly the approximation fails for in this instance. This is characteristic of the single-source solution when the first layer's thickness is less than one transport mean free path. This is because the single-source approximation does not take into account the second layer's contribution to the reflected light.

The two-source approximation reflectance closely follows the Monte Carlo results for an optically thin layer with and in figure 6, we see that it has an error of less than 5%. even though the previous approximation fails. This means that the two-source solution effectively reduces our error's dependency on the layer depth.

4. CONCLUSIONS

This paper has laid out an improved method for solving the diffusion approximation for light traveling through multiple layers. The method was illustrated by deriving the diffusion approximation for the specific case of a two-layer, turbid medium. A collimated, incident beam was replaced by one equivalent isotropic point in each layer. These sources' locations and strengths were based on their layer's optical properties. The resulting diffusion equations were then solved by using a two-dimensional Fourier transform to get them in to ordinary differential equation form. We then used the Simpson's quadrature take the inverse Fourier transform and get the fluence of light through the medium. Then using equation 15, we converted the fluence at z=0 into reflected light. The results were then compared against the results of previous solutions. We also briefly addressed methods for extending the solution to x layers using x sources, where x is a positive, finite integer.

Figure 3 shows both the approximations agree with the Monte Carlo simulations for an optically thick first layer. We also see that the accuracy region of the two-source approximation is dependent on both layers where as the single-source's solution only depends on the top layer. In Figure 5 we see that the previous solution completely breaks down for layer thicknesses less than $1/\mu_{t1}'$ while the two-source approximation stays within a 5% error bound.

REFERENCES

1. T. .J. Farrell and M. S. Patterson, "A diffusion theory model of spatially resolved, steady-state diffuse reflectance for the noninvasive determination of tissue optical properties *in vivo*," Med. Phys. 19, 879 - 888 (1972)

2. L.-H. Wang and S. L. Jacques, "Use of a laser beam with an oblique angle of incidence to measure the reduced scattering coefficient of a turbid medium," Applied Optics 34, 2362-2366 (1995).

3. A. Kienle, M.S.Patterson, N.Dognitz, R.Bays, G.Wagnieres, and H. Van Den Bergh, "Noninvasive determination of the optical properties of two-layered turbid media," Appl. Opt 37, 779-791 (1998).

4. R.C. Haskell, L.O. Svaasand, T.T. Tsay, T.C. Feng, M. McAdams, and B.J. Tromberg, "Boundary Conditions for the diffusion equation in Radiative Transfer," J. Opt. Soc. Am A, 11, 3737-3741 (1994).

5. M. N. O. Sadiku, "Finite Difference Methods," in *Numerical Techniques in Electromagnetics, 2nd edition*(CRC Press, Boca Raton, Florida, 2001) pp 197-199.

[6] 6. G. Alexandrakis, T.J. Farrell, M.S. Patterson, "Accuracy of the diffusion approximation in determining the optical properties of a two-layer turbid medium," Appl. Opt. 37, 7401-7409 (1998)

7. L.-H. Wang, S. L. Jacques, and L.-Q. Zheng, "MCML - Monte Carlo modeling of photon transport in multi-layered tissues," Computer Methods and Programs in Biomedicine 47, 131-146 (1995).