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Contents lists available at ScienceDirect

# Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: [www.elsevier.com/locate/jqsrt](http://www.elsevier.com/locate/jqsrt)

## Note

# Light propagation in turbid media: A generalization of the solution given by the diffusion approximation, based on the moments of multiple scattering

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## ARTICLE INFO

### Article history:

Received 17 December 2009

Received in revised form

15 July 2010

Accepted 16 July 2010

### Keywords:

Turbid media

Diffusion approximation

Biomedical optics

## ABSTRACT

In this work we propose a generalization of the solution for light propagation in turbid media given by the diffusion approximation (DA), based on the calculus of the photon coordinates momenta. The main results of the proposed approach are: (1) the contributions of the scattering coefficient  $\mu_s$  and the anisotropy factor  $g$  are explicitly separated, and (2) the minimum number of collisions  $N$  for which the DA is valid can be inferred. We demonstrate that when the number of collisions,  $N$ , is large our solution tends to that of the diffusion equation, but for those cases with small  $N$  or when the absorption coefficient,  $\mu_a$ , cannot be considered as much smaller than the reduced scattering coefficient,  $\mu_s'$ , our solution remains useful. Validation using Monte Carlo simulations, taken as a standard, is presented for both situations. Comparisons with results from other authors are also provided.

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## 1. Introduction

Photon propagation inside turbid media is described by the radiative transfer equation (RTE)<sup>1</sup> [1,2]. It contains three optical parameters, namely the refractive index  $n$ , the scattering coefficient,  $\mu_s$  and the absorption coefficient,  $\mu_a$ . When the number of interactions of the photon with the medium is large enough, the RTE can be replaced by the diffusion approximation (DA). In this case, the new parameter  $\mu_s' \equiv \mu_s(1-g)$ , being  $g = \langle \cos\theta \rangle$  the mean value of the cosine of the polar scattering angle,  $\theta$ , can be defined. Conditions for validity of the DA are that the

characteristic dimension of the medium,  $d$ , must satisfy  $d \gg 1/\mu_s'$ , and that  $\mu_a \ll \mu_s'$ .

In this work we construct a solution for infinite media that expands the solution for the DA being still valid if the conditions mentioned above do not hold. The mean values and the dispersion of the photons path lengths remain expressed in terms of  $\mu_s, \mu_a$  and  $g$ , showing the individual contributions of  $\mu_s$  and  $g$  to  $\mu_s'$ . In this way, for a given number of collisions,  $N$ , it holds  $N/\mu_s \approx vt$ , where  $1/\mu_s$  is the mean free path between collisions and  $v$  is the speed of light inside the medium,  $v = c/n$ . Our approach retrieves the solution of the DA for high number of collisions, calculating for which values of  $N$  the conventional solution for the DA is valid. It must be stressed that even though we treat only the case of the diffusive photons (in the sense that  $g$  is strictly  $< 1$ ), our solution also includes the cases for which  $N$  is not very large and when the condition  $\mu_a \ll \mu_s'$  is not satisfied. Additionally, we show that the distribution of path lengths containing most of the photons, (the diffusive pulse) starts at  $t > r/c$ , as

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<sup>1</sup> The concept of "photon" is used here in a phenomenological sense and what is meant by "photon" is a discrete packet of energy which is launched to study the moments of the distribution in light propagation when multiple scattering is present.

expected for diffusive photons. The proposed solution is based on some articles in which the moments of multiple scattering are calculated [3–5]. Even though it is well known that for a few number of collisions, effects of polarization may be of relevance, we will not address this issue in this contribution, along the lines of Ref. [6].

Our contribution is organized as follows: in Section 2, we present a brief review of the moments of the path lengths distribution, we introduce our main assumptions and treat two special cases. In Section 3, our general formula is constructed and we discuss the generalization with respect to DA, showing some validations by comparison with Monte Carlo simulations. Finally, we present the main conclusions.

## 2. Moments of multiple scattering

Refs. [3–5] make use of probabilistic models to calculate the moments of the path length distribution when multiple scattering is present. Since the results given by these authors are essentially equal, we will choose the presentation of Ref. [5] because of its simplicity.

The basic idea is summarized in the following. If every single photon is launched in direction  $z$  and in its first step it covers a distance  $l_0$ , successive positions of the photon will be given by consecutive use of the Euler angles matrix (with the choice of the azimuthal angle  $\phi = 0$ , see Fig. 1). Thus, first and second expectation values can be calculated. The main results will be written in terms of the number of collisions,  $N$ ; they may be expressed as a function of time by the relation  $N = \mu_s vt$ , being  $v$  the speed of light in the medium. These results are:

R 1. *First order moments:* For photons launched along the  $z$  axis, the first moments for the spatial coordinates, which can be physically taken as the coordinates of the center of the photons “cloud” are given by

$$\langle z_N \rangle = \frac{1}{\mu_s} \frac{1-g^N}{1-g}, \quad \langle x_N \rangle = 0, \quad \langle y_N \rangle = 0. \quad (1)$$

From the former equation we can get these first moments that, for the case  $N \gg 1$  results, taking into

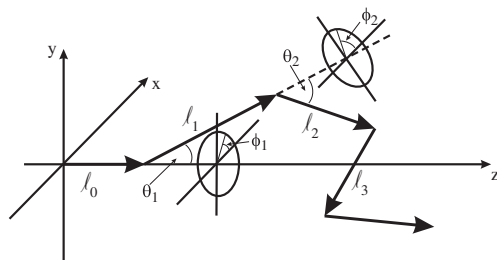


Fig. 1. Schematic drawing of scattering in a random medium; the source emits a thin light beam in the  $z$  direction. The step lengths taken by the photons are symbolized by the vector lengths,  $l_j$ . At each scattering position, a new azimuthal angle,  $\phi$ , and a new polar angle,  $\theta$ , are required.

account that for  $g < 1$ ,  $(1-g^N)/(1-g) \approx 1/(1-g)$ , that is

$g$	$< 1$	$1$
$\langle z_N \rangle$	$1/\mu_s'$	$\frac{N}{\mu_s}$
$\langle x_N \rangle, \langle y_N \rangle$	$0$	$0$

R 2. *Second order moments:* The corresponding second order moments,  $m_2$ , from which the variances  $\sigma^2 = m_2 - m_1^2$  can be calculated are, in terms of  $N$ , given by

$$\langle z_N^2 \rangle = \frac{2}{3\mu_s^2(1-g)} \left[ N - \frac{1-g^N}{1-g^2} (-2+g+g^2+2g^{N+1}) \right], \quad (3)$$

and

$$\langle x_N^2 \rangle = \langle y_N^2 \rangle = \frac{2}{3\mu_s^2(1-g)} \left[ N - \frac{1-g^N}{1-g^2} (1+g+g^2-g^{N+1}) \right]. \quad (4)$$

Now the limiting values are, for  $N \gg 1$ , and taking into account that for  $g < 1$ ,  $(1-g^N)/(1-g^2) \approx 1/(1-g^2)$ :

$g$	$< 1$	$1$
$\langle z_N^2 \rangle$	$\frac{2N}{3\mu_s^2(1-g)}$	$\frac{N^2}{\mu_s^2}$
$\langle x_N^2 \rangle = \langle y_N^2 \rangle$	$\frac{2N}{3\mu_s^2(1-g)}$	$0$

R 3. *Variances:* With the values obtained above it is now possible to find the variances for every set of parameters  $\mu_a, \mu_s, g$  and  $N$ ; this will be used later to build up the most general expression of our proposed solution (given in Eq. (8)). The photons cloud propagating inside the medium can thus be interpreted as an ellipsoid centered at coordinates  $(\langle x_N \rangle, \langle y_N \rangle, \langle z_N \rangle)$  with semi-axes  $\sigma_x, \sigma_y, \sigma_z$  given by the square roots of the corresponding variances:  $\sigma_z = [\langle z_N^2 \rangle - \langle z_N \rangle^2]^{1/2}$  and  $\sigma_x = \sigma_y = [\langle x_N^2 \rangle]^{1/2}$ . For  $N \gg 1$ , and  $0 \leq g < 1$ , longitudinal and transverse axes are equal, that is,  $\sigma_z = \sigma_x = \{2N/[3\mu_s^2(1-g)]\}^{1/2}$ .

The case  $g=1$ : Expressions (2) are of utmost importance for the solution presented in this work, since from its interpretation we can introduce the following two physically grounded assumptions: first, this equation tell us that  $g=1$  refers to ballistic photons, and thus, this is equivalent to think that the proposed model implicitly contains a ballistic peak at position  $r = vt (\equiv N/\mu_s)$ . That means that in our solution we can include a term with a Dirac delta function,  $\delta(t-r/v)$ , for the ballistic photons, as it is done by Paasschens, who solved analytically the radiative transfer equation [6]. Second, it is possible to assess without any loss of thoroughness that, provided that, diffusive photons will arrive at any point  $r$  after the ballistic ones, the solution will contain for this second kind of photons a Heaviside function,  $H(t-r/v) \rightarrow H(N-\mu_s r)$ . In practical applications, the ballistic photons are of little importance because, for a given propagation distance  $r$ , their number decays as  $e^{-(\mu_a + \mu_s)r}$ , and diffusive photons are present in the most important proportion.

### 3. Construction of a generalized formula for infinite media

Our goal is to construct a formula that, for the simplest case of an infinite medium and for  $N \gg 1$  (or for long  $t$ ), tends to the known solution for the DA. To our end we take into account that for  $N \gg 1$  and  $g < 1$  (i.e., the diffusive photons) the probability density will take the Gaussian form predicted by the law of large numbers:

$$\lim_{N \gg 1} W(x,y,z; N) = \frac{e^{-(\mu_a/\mu_s)N}}{(2\pi\sigma^2)^{3/2}} \exp\left(-\frac{x^2+y^2+(z-\langle z_N \rangle)^2}{2\sigma^2}\right) m^{-3}, \quad (6)$$

where  $\langle z_N \rangle = 1/[\mu_s(1-g)]$  and  $\sigma^2 = 2N/[3\mu_s^2(1-g)]$ .

Generalizing for all values of  $N$  and  $g$ , it is then possible to write, for photons incident in the  $z$  direction, and taking into account that their behavior in directions  $x$  and  $y$  is identical (that is  $\sigma_x^2 \equiv \sigma_y^2$ ),

$$\frac{W(x,y,z; N)}{m^{-3}} = \frac{e^{-(\mu_a/\mu_s)N}}{(2\pi\sigma_x^2)} \exp\left(-\frac{x^2+y^2}{2\sigma_x^2}\right) \frac{1}{(2\pi\sigma_z^2)^{1/2}} \exp\left(-\frac{(z-\langle z_N \rangle)^2}{2\sigma_z^2}\right), \quad (7)$$

where the values of  $\langle z_N \rangle$ ,  $\sigma_x^2 \equiv \sigma_x^2(N, \mu_s, g)$  and  $\sigma_z^2 \equiv \sigma_z^2(N, \mu_s, g)$  are given in Eqs. (1), (3), and (4), respectively. Note that the mean value  $\langle z_N \rangle$  in the last exponential function is irrelevant for infinite media, but it is of utmost importance if dealing with semi-infinite or slab geometries.

As stated above, when stressing the importance of Eq. (2), diffusive photons will arrive at a given position  $r=(x^2+y^2+z^2)^{1/2}$  later than the ballistic ones: there are no diffusive photons detected until  $t \geq r/v(N \geq \mu_s r)$ ; it is thus necessary to include a Heaviside function,  $H(N-\mu_s r)$ , accounting for this fact. It should be noted that this statement is not introduced *ad-hoc*, but is the result of the analysis of Eq. (2). Then, the complete solution, for all values of  $g$ , takes the form

$$\frac{\Phi_i(x,y,z; N)}{m^{-2}s^{-1}} = \frac{v \exp\left[-\left(\frac{x^2+y^2}{2\sigma_x^2} + \frac{(z-\langle z_N \rangle)^2}{2\sigma_z^2}\right)\right]}{(2\pi\sigma_x^2)(2\pi\sigma_z^2)^{1/2}} H(N-\mu_s r) \exp(-\mu_a N/\mu_s), \quad (8)$$

with  $\sigma_z^2$  and  $\sigma_x^2$  given, as already mentioned, by Eqs. (3) and (4), respectively.

It is known that the Gaussian distribution (8) is valid for large  $N$ ; however, comparison of our results with those from Paasschens [6], shows that for the case where the optical parameters are similar to those of biological tissues and for a thickness as thin as  $z=2$  mm, both results agree within 10% for  $N \geq 10$  and, for  $z=4$  mm, they agree within 5% for  $N \geq 6$ . Both situations are clearly not represented by the DA. It is important to remark that, even though we treat only the diffusive photons ( $g < 1$ ), our solution is more general than the one provided by Eq. (6); this is based on both the presence of the function  $H(N-\mu_s r)$  and the different expressions for  $\sigma_x^2$  and  $\sigma_z^2$ .

### 3.1. The diffusive photons; comparison with the solutions given by the diffusion approximation

It can be shown that Eq. (8) describes all type of scattering of photons in turbid media, included those known as ballistic and snake. While for turbid media of biological interest, those are not of importance, diffusive photons constitute the greater proportion of all detected ones. Accordingly to our model, they follow the law given in Eq. (8) for  $g < 1$ .

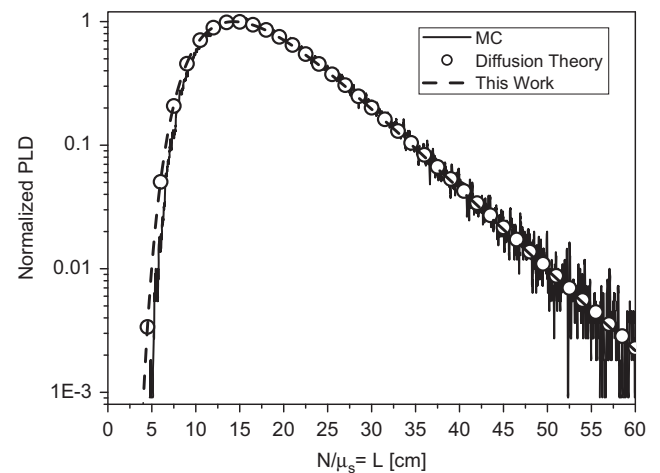
#### 3.1.1. The case $\mu_a \ll \mu_s'$

It is interesting to compare the values of  $\Phi_i$  given by our Eq. (8) and those given by the DA. It is verified that for small values of  $z$  there is a clear discrepancy between both solutions (see below); however, as  $z$  becomes larger both solutions tend to the same values inside the whole interval of  $N/\mu_s$  (or equivalently,  $vt$ ). To introduce a quantitative criterion, let us consider  $\mu_s$  and  $g$  similar to those found in biological tissues. For this case ( $\mu_s' \gg \mu_a$ ), when the distances between source and detector satisfy  $d \geq 8/\mu_s'$ , the maxima of both distributions are almost coincident [7,8]. As an example, in Fig. 2, we compare the MC outcomes with both the values from the diffusion approximation and from this work for a distance between source and detector  $d=30$  mm. The parameter values are:  $\mu_a = 0.01$  mm<sup>-1</sup>,  $\mu_s = 5$ ,  $g=0.8$ ,  $\mu_s' = 1$  mm<sup>-1</sup> and  $n=1$ .

On the contrary, for values of the absorption coefficient,  $\mu_a$ , much greater than those found in biological tissues, this coincidence is lost and both the solutions differ because the DA is no longer valid, whereas our solution is useful. This fact will be shown immediately below.

#### 3.1.2. The combined case: $d < 8/\mu_s'$ and $\mu_a \lesssim \mu_s'$

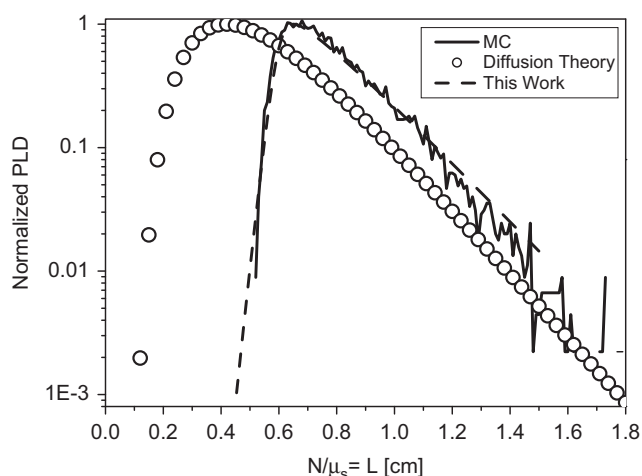
For the cases involving biological tissues, the absorption coefficient ranges from  $\mu_a \approx 0.005$  mm<sup>-1</sup> for normal tissues to approximately  $\mu_a \approx 0.03$  mm<sup>-1</sup> for tumors,



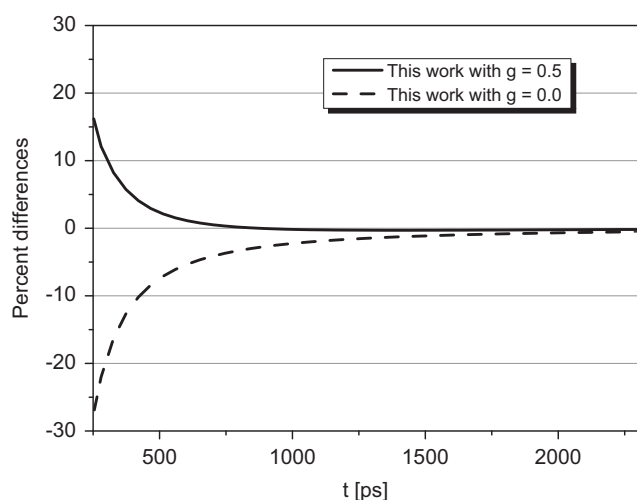
**Fig. 2.** Comparison of the normalized path lengths distribution (PLD) when the diffusion approximation holds:  $d=30$  mm ( $> 8/\mu_s'$ ),  $\mu_a = 0.01$  mm<sup>-1</sup>,  $\mu_s = 5$ ,  $g=0.8$ ,  $\mu_s' = 1$  mm<sup>-1</sup> and  $n=1$ . Note that for this case both, diffusion theory and our proposal, fit well the Monte Carlo outcome, which is taken as a validation standard.

while the reduced scattering coefficient is about  $\mu_s' \approx 1 \text{ mm}^{-1}$  (see for example [2]). Thus, for biological applications, the condition  $\mu_a \ll \mu_s'$  required by the DA is always satisfied.

On the other hand, our solution allows to visualize what happens for cases in which  $\mu_a < \mu_s'$  (but not  $\mu_a \ll \mu_s'$ ). In Fig. 3, we present the case where there are two exceptions to the validity of the DA:  $d < 8/\mu_s'$  and  $\mu_a \lesssim \mu_s'$ . In effect, now  $d=5 \text{ mm}$  and  $\mu_a = 0.5 \text{ mm}^{-1}$ ; the other parameters are as presented in Fig. 2. Note that, whereas the DA makes nonsense, because it shows non-physical photons for  $N/\mu_s < d$  (or  $t < d/v$ ), our solution and the MC outcomes are nearly coincident.



**Fig. 3.** Comparison of the normalized path lengths distribution (PLD) when the diffusion approximation does not hold:  $d = 5 \text{ mm} (< 8/\mu_s')$  and  $\mu_a \lesssim \mu_s'$ . The optical parameters are:  $\mu_a = 0.5 \text{ mm}^{-1}$ ,  $\mu_s = 5$ ,  $g = 0.8$ ,  $\mu_s' = 1 \text{ mm}^{-1}$  and  $n = 1$ . Note that, whereas our proposal still fits Monte Carlo values, diffusion theory fails to reproduce them, for  $L < d$ .



**Fig. 4.** Comparison of the DA with the results of this work, in terms of the percent difference. Light transmittance is considered inside a 4 cm thick nonabsorbing slab with  $\mu_s' = 2 \text{ cm}^{-1}$  and  $n = 1.4$ . The solid line corresponds to the results of Eq. (9) when  $g = 0.5$  and the dashed line represents the case for  $g = 0$ . This results must be compared with Fig. 6 in Ref. [9].

### 3.2. Comparison with MC outcomes from other authors

As a complementary validation of our procedure for physical conditions far from those required by the DA, we present in Fig. 4 the percent difference,

$$\frac{\text{Eq. (8)} - \text{DA}}{\text{DA}} \quad (9)$$

for a 4 cm thick, nonabsorbing slab with  $\mu_s' = 2 \text{ cm}^{-1}$ ,  $n = 1.4$  and for two values of the anisotropy factor, namely  $g = 0.0$  and  $0.5$ . In this figure it can be seen that for short times,  $< 500 \text{ ps}$ , there is no agreement between DA and our approach. Moreover, the discrepancy depends on the value of  $g$ , being positive for  $g = 0.5$  and negative for the isotropic case,  $g = 0$ . For larger times, the percent error rapidly tends to values  $< 5\%$ . This result should be compared to that of Fig. 6 in the paper by Martelli et al. [9], where the same calculation as in Eq. (9) is shown, but using Monte Carlo simulations instead of the result of Eq. (8). The agreement between both figures is very remarkable.

### 4. Conclusions

In this contribution we have constructed, starting with the first and second moments of the path length distributions, an improvement with respect to the solution given the DA, presented in terms of the path lengths,  $N/\mu_s$  (or, equivalently, in terms of  $ct$ ). In our proposal, the independent contributions of  $\mu_s$  and  $g$  are evident in Eqs. (1), (3) and (4); for  $N \gg 1$  it naturally happens that  $\mu_s' = \mu_s(1 - g)$ .

We have verified that our approach produces values in accordance with the MC outcomes even in the case where there are two strong exceptions to the validity conditions of the DA:  $d < 8/\mu_s'$  and  $\mu_a \lesssim \mu_s'$  (Fig. 3). Therefore, the importance of the proposed solution is not restricted to the biomedical optics field.

### Acknowledgements

The authors would like to acknowledge financial support from Grant PICT 38058 from ANPCyT.

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