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Analysis of the applicability of the classical probabilistic parameters of the Monte Carlo algorithm for problems of light transport in turbid biological media with continuous absorption and discrete scattering

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Abstract. **Simulation of light propagation by the statistical Monte Carlo (MC) method is widely used in many fields, especially in astrophysics, atmospheric optics, ocean optics, and nuclear medicine. In the optics of biological tissues, the MC method is used to simulate the luminous flux, which is formed during various medical therapeutic or diagnostic procedures inside a biological tissue and on its surface. In such calculations, the MC method is commonly considered as a reference one, which ensures an arbitrarily high accuracy with an increase in the number of 'photons'. However, it can be shown that this is not always the case. In this paper, in the methodological aspect, the idealised one-dimensional problems of the transport theory for a turbid medium with continuous absorption and scattering and a turbid medium with discrete scatterers inside a continuously absorbing medium are considered. Their exact analytical solutions are presented and compared with the results of statistical modelling by the MC method. It is found that the use of classical probabilistic parameters for a medium with continuous absorption and scattering in the MC algorithm leads to a systematic method error in determining the values of radiation fluxes for biological media with discrete scattering, up to 10% for fluxes at the boundary in some cases. The causes of the error are discussed and it is shown how to modify the probabilistic parameters of the MC algorithm to eliminate it.**

Keywords: *light propagation, turbid medium, biological tissue, transport theory, Monte Carlo method, scattering coefficient, absorption coefficient, albedo.*

1. Introduction

As a rule, any tomographic or spectrophotometric diagnostic problems in biology and medicine are associated with the solution of inverse problems [1, 2]. The accuracy of the solution of inverse problems is primarily determined by the accuracy of the formulation and solution of the direct problem.

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For spectrophotometric problems, the most used analytical theory today, describing the propagation of light in turbid (light-scattering) media at the macrolevel, is the photometric (kinetic) transport theory (TT), ideologically based on the Boltzmann kinetic equation. It was substantiated and developed in the XX century in the classical papers by Khvolson, Kubelka–Munk, Gurevich, Milne, Chandrasekhar, Ambartsumyan, Ishimaru and many other authors (see, e.g., [3–6]). However, no exact analytical solution of the general integral-differential radiation transfer equation (RTE) in closed form has been found. Therefore, at the end of the 20th century, with the creation of powerful computers, the main attention of researchers switched to a statistical numerical method for calculating optical fields, the Monte Carlo (MC) method (see, e.g, [7–10]). In biotissue optics, the MC method in most cases is understood today as statistical modelling of a probabilistic walk of a conditional 'photon' – a classical, non-quantum, object (analogue of a zero-size gas molecule), or a packet of such photons – inside a biological tissue. In this case, the random free paths of photons, the probabilities of their scattering and absorption in the medium are closely related to the TT and depend on the deterministic radiation absorption coefficient in the medium, the albedo of single scattering (SS) and the phase scattering function (for spatial problems) [9, 10].

It is important to note here that the classical photometric RTE is originally formulated for a macroscopically isotropic medium under the assumption that it a priori has certain averaged coefficients of absorption (μ_a) and scattering (μ_s) (with the dimension cm^{-1}) independent of each other. The medium microstructure and the methods for obtaining these coefficients are usually not considered in the foundations of the theory [4–6]. The coefficients are considered to be given. This is mathematically equivalent to an idealised medium that continuously absorbs and scatters light as it propagates along any infinitely small segment dx of the path, which yields equations for a smooth brightness function. Later (or in parallel), RTE was successfully used in the physics of ionising radiation to describe scattering by particles (atoms, electrons, protons) – spatially discrete structures (centres) that scatter and absorb light. Today, such problems of scattering by particles are routine, e.g., in radiation medicine. However, in the optical range of the spectrum, biological tissues and media are continuous absorbers, but discrete scatterers [10, 11]. The absorption of light can be assumed occurring continuously throughout the thickness of the biological tissue in accordance with the Bouguer exponential law, while the scattering takes place only on inhomogeneities of its cellular structure, which are spaced discretely within the absorbing medium. Therefore, it is natural to pose a question of how correct it is to use the probabilistic parameters of a continuous medium in the MC algorithm, as generally accepted in biomedical optics, when considering media with continuous absorption but discrete scattering. It seems that this question has not come to the attention of researchers until recent time.

Recently, in [12,13], we showed by particular examples the presence of discrepancies between the results of numerical simulations by the MC method with the classical probabilistic parameters of a continuous medium and exact analytical solutions of differential TT equations for the same initial problems, but for a medium with continuous absorption and discrete scattering. The purpose of this work is to show the methodological differences in the formulation of problems and in the determination of the probabilistic parameters for the MC method in the case of media with continuous and discrete scattering and continuous absorption of radiation.

2. Preliminary remarks to the formulation of model problems

Since we are considering the methodological issue of discrepancies in the formulation of problems and in their solutions for media with continuous and discrete scattering, it is easiest to do this by the example of the simplest one-dimensional (1D) problems, for which there are exact and illustrative analytical solutions in a closed form [3, 5, 11, 12, 14]. Although 1D problems seem to be far from the real physical world, they are the basis for the phenomenological substantiation of the Bouguer exponential law in photometry [15] and were repeatedly used in the works of Schuster, Schwarzschild, Gurevich, Kubelka, Munk and other authors [5, 6]. Therefore, methodologically, 1D problems are reasonably substantiated in TT and, moreover, have a number of advantages. These problems not only have exact analytical solutions that can be easily analysed, but also remove the problem of taking into account the wave properties of electromagnetic radiation in TT, which are often argued about, because no transverse wave is realisable in 1D space. Only the basic photometric formulation of the ray problem remains. The phase scattering function is also excluded from consideration. In the 1D problem, it degenerates into a single value of the coefficient of back reflection (scattering) of radiation from the boundaries of inhomogeneities inside the medium. It is important to emphasise that the above applies only to truly 1D problems, in which light propagates in the form of an infinitely thin ray along a single X axis. It is exactly these problems that will be considered below.

Sometimes in TT, 1D problems are understood as propagation of a wide collimated beam of light (in electrodynamics, a plane electromagnetic wave), as, e.g., in the classical Milne problem [4, 6]. Another example is the problem of projecting 3D light propagation onto a single axis, which was solved by Kubelka and Munk, with the formulation of an additional closing condition [5]. These tasks are reduced to solving 1D problems. However, we will not consider them here, since solving these problems is more complicated and not so clear. We are only interested in the simplest phenomenological formulation of the ray energy (photometric) stationary problem of the transfer of power (energy) of radiation by an infinitely thin beam along one single X axis (there are neither other axes, nor angular scattering). The MC method can also be easily implemented and justified for such 1D problems. This simplifies the problem. If there is a fundamental methodological difference in the formulation and solution of problems for media with continuous and discrete scattering, it is expected to manifest itself immediately in such idealised 1D problems, without complicating them with other directions of radiation propagation, phase scattering functions, etc. The nonstationarity will be also an unnecessary complication, and taking it into account should not lead to fundamentally different results.

3. Model problems in the single scattering approximation

3.1. Continuous medium with continuous absorption and continuous scattering

Let us first consider the classical TT problem of light propagation in a continuous medium with continuous absorption and continuous scattering in the SS approximation (Fig. 1). The SS approximation also simplifies the formulation and solution of the problem. It means that a light beam with power F_0, penetrating from the outside into a turbid medium, as it propagates in the positive direction of the X axis inside the medium, permanently and irreversibly loses part of its power on each elementary segment of the path dx due to absorption and scattering. The light flux inside the medium, $F_+(x)$, will be a coordinate function sought. The backward flux $F_-(x)$ formed by scattering of the flux $F_+(x)$ in the medium propagates in the opposite direction of the X axis, but is no longer scattered. It can only lose power through absorption. In a word, any photon in the flux $F_+(x)$, once elastically scattered and having changed its direction to the opposite, in the reverse flux $F_-(x)$ no longer experiences scattering and can only be absorbed. The medium where the radiation propagates is characterised by generally accepted deterministic optical properties, the absorption μ_a and scattering μ_s coefficients, independent of each other and considered to be known. These coefficients do not necessarily coincide with those for real 3D media*.

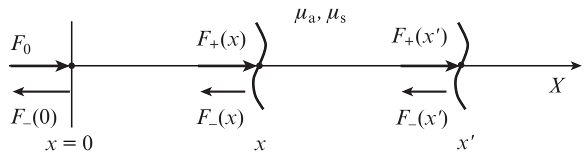

Figure 1. Statement of the 1D problem in the SS approximation for a medium with continuous absorption and continuous scattering.

The exact solution to this problem has long been known (see, e.g., [16]). The system of differential equations

$$\begin{aligned} \frac{dF_+(x)}{dx} &= -(\mu_a + \mu_s)F_+(x) , \\ \frac{dF_-(x)}{dx} &= \mu_a F_-(x) - \mu_s F_+(x) \end{aligned} \quad (1)$$

is solved, which is phenomenologically 'derived' (in fact, postulated) in TT, based on simple logical considerations that the

*When obtaining the closing condition, Kubelka and Munk, for example, showed that there might be a difference in the interpretation of such coefficients for 3D and 1D problems [5].

direct flux $F_+(x)$, as it propagates, is absorbed and scattered at the path segment dx, whence the first equation of the system follows (if we assume the independence of the acts of scattering and absorption). The reverse flux $F_-(x)$, formed without losses during the scattering of the flow $F_+(x)$ (the second term on the right-hand side of the second equation), is then only absorbed (the first term on the right-hand side of the second equation). Let us present the solution of system (1) with the simplest boundary conditions for a semi-infinite medium without taking into account the reflection at the outer boundary: $F_+(x) = F_0$, $F_-(\infty) = 0$ [16]. Under such boundary conditions, the sought forward flux has the form of an exponentially decaying function similar to the Bouguer law:

$$F_+(x) = F_0 \exp[-(\mu_a + \mu_s)x], \tag{2}$$

and the reverse flux is found by integration:

$$F_-(x) = \int_x^\infty \exp[-\mu_a(x' - x)]\mu_s F_+(x')\,dx'. \tag{3}$$

The flux $F_-(x)$ also decays exponentially with increasing x:

$$F_-(x) = F_0 \frac{\mu_s}{2\mu_a + \mu_s} \exp[-(\mu_a + \mu_s)x]; \tag{4}$$

however, as it propagates back to the illuminated 'surface', it tends to increase due to the contribution of the scattered component of the flux $F_+(x)$.

Application of the classical MC method to such a problem yields a solution that ideally coincides with the exact analytical solutions (2) and (4). When constructing an MC simulation algorithm, the main difficulty is to express the probabilistic parameters of the model in terms of the physical optical properties of a turbid medium. For the 1D problem and the SS approximation, there are three such parameters: two photon mean free paths in the forward and backward directions (l_+ and l_-, respectively) and the photon scattering probability P_s. In biomedical optics, they are usually specified in the MC algorithm in the following ('classical') way. The classical scattering probability P_s^{cl} is equated to the SS albedo [7, 17]:

$$P_s^{cl} = \frac{\mu_s}{\mu_a + \mu_s}. \tag{5}$$

In this case, the connection between expression (5) and Eqns (1)–(4) is usually not explained in the papers, but is considered *a priori* clear. The random value of the photon free path length l_+^{cl} inside the flux $F_+(x)$ is calculated at each iteration step by generating a random number ξ_1 uniformly distributed over the segment [0; 1] according to the formula

$$l_+^{cl} = -\frac{\ln \xi_1}{\mu_a + \mu_s}, \tag{6}$$

taking into account the exponential probability distribution function for l_+^{cl}.

To understand further conclusions, it is methodologically important to emphasise that the form of the probability distribution function for l_+^{cl} [exponential, as follows from Eqn (2)] must be known to obtain and substantiate Eqn (6). For the reverse flux (for l_-), a different formula is required. The difference is determined by the logic of the SS approximation. The flux $F_-(x)$ in the SS approximation is not scattered, so for it $\mu_s = 0$. Then, by analogy with Eqn (6), we use the expression

$$l_-^{cl} = -\frac{\ln \xi_2}{\mu_a}, \tag{7}$$

where ξ_2 is the generated random number, uniformly distributed on the interval [0; 1], like ξ_1.

A comparison of the exact analytical solution with the numerical one, obtained by the MC method, for fluxes inside and on the surface of such a continuous 1D medium is shown in Fig. 2. The complete coincidence of the solutions is obvious here. It is described in many basic textbooks.

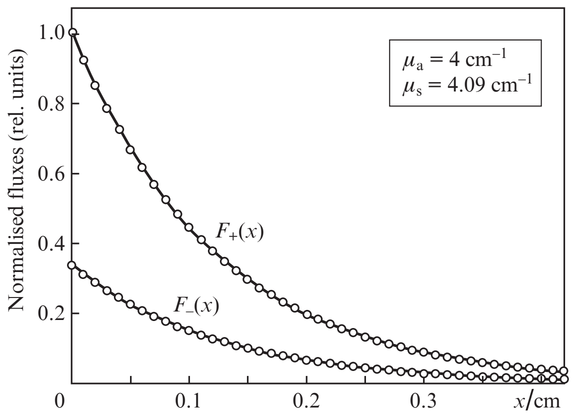

Figure 2. Numerical solutions by the MC method (circles) and analytical solutions (solid curves) of the 1D problem in the SS approximation for a medium with continuous absorption and continuous scattering. The values of the fluxes $F_+(x)$ and $F_-(x)$ are normalised to F_0.

3.2. Medium with continuous absorption and discrete scattering

When considering discrete scatterers inside a continuously absorbing 1D medium, the analytical solution of the problem is not so obvious, although it is also known [11, 14]. The first difficulty arises here with determining the value of μ_s. Each single ith scatterer (inhomogeneity) inside such a turbid medium scatters (reflects) back a certain fraction of the incident radiation $R_i \leqslant 1$ (for example, this is an analogue of the Fresnel reflection coefficient R). How to find μ_s if the concentration of inhomogeneities in the medium μ_ρ is known? The classical monograph [5] gives an intuitive expression $\mu_s = \mu_\rho R$. However, it can be shown that this is not entirely true.

Following Ref. [14], let us consider the interval Δx inside such a 1D medium, which contains N identical scattering inhomogeneities (Fig. 3). Let the distance between them be the same and equal to $\Delta x/N$ *. Without loss of generality, we also assume that all R_i = const = R, and the distances between the extreme inhomogeneities and the boundaries Δx are $\Delta x/(2N)$. This formulation of the problem and the structure of the Δx interval simplify the final analytical solutions and their derivation. In particular, to derive the differential equation for the flux $F_+(x)$, it suffices to consider the limit

$$\frac{dF_+(x)}{dx} = \lim_{\Delta x \to 0} \frac{\Delta F_+(x)}{\Delta x} = \lim_{\Delta x \to 0} \frac{\Delta F_+(x + \Delta x) - F_+(x)}{\Delta x}. \tag{8}$$

* It is not difficult to show that random distances, for example, with a normal distribution around $\Delta x/N$, will give, on the statistically average, a similar result.

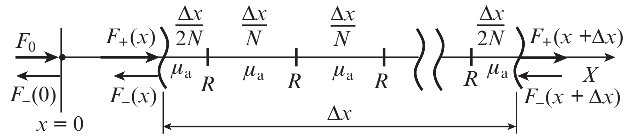

Figure 3. Statement of the 1D problem in the SS approximation for a medium with continuous absorption and discrete scattering.

Noting that

$$F_+(x+\Delta x) = F_+(x)\exp(-\mu_a \Delta x)(1-R)^N, \tag{9}$$

using for the concentration of inhomogeneities the definition [11, 14]

$$\mu_\rho = \lim_{\Delta x \to 0} \frac{N}{\Delta x}, \tag{10}$$

and disclosing the 0/0 uncertainties in Eqn (8), we easily come to a differential equation identical to the first equation of system (1), if we introduce the notation

$$\mu_s = -\mu_\rho \ln(1-R). \tag{11}$$

Note that Eqn (11) differs from the expression $\mu_s = \mu_\rho R$ proposed by Ishimaru and tends to it only for $R \ll 1$. However, if we substitute μ_s (11) into the first equation of system (1), then the differential equations for $F_+(x)$ turn out to be identical in both cases.

Deriving the differential equation for $F_-(x)$ is somewhat more complicated. The flux $F_-(x)$ consists of two parts. The first part is the flux $F_{\Sigma\,\Delta x}(\Delta x)$ backscattered from the segment Δx, while the second part is the flux $F_-(x+\Delta x)$ that passed from right to left through the segment Δx and was attenuated due to absorption. Mathematically, this can be represented as

$$F_-(x) = F_{\Sigma\,\Delta x}(\Delta x) + F_-(x+\Delta x)\exp(-\mu_a \Delta x). \tag{12}$$

To find $F_{\Sigma\,\Delta x}(\Delta x)$, it is necessary to take into account the scattering from all inhomogeneities in the segment Δx. For the first inhomogeneity, we can write the expression

$$F_1^-(\Delta x) = F_+(x)\exp(-\mu_a \Delta x/N)R, \tag{13}$$

for the second

$$F_2^-(\Delta x) = F_+(x)\exp(-\mu_a \Delta x/N)(1-R)\exp(-2\mu_a \Delta x/N)R$$
$$= F_1^-(\Delta x)\exp(-2\mu_a \Delta x/N)(1-R). \tag{14}$$

Then for the Nth inhomogeneity, we will have the relation

$$F_N^-(\Delta x) = F_1^-(\Delta x)\exp[-2\mu_a (N-1)\Delta x/N](1-R)^{N-1}. \tag{15}$$

The sum of all $F_i^-(\Delta x)$ is a sum of a geometric progression, therefore $F_{\Sigma\,\Delta x}(\Delta x)$ can be easily found in explicit form:

$$F_{\Sigma\,\Delta x}(\Delta x) = \sum_{i=1}^{N} F_i^-(\Delta x) = F_1^-(\Delta x)$$
$$\times \frac{1-[\exp(-2\mu_a \Delta x/N)(1-R)]^N}{1-\exp(-2\mu_a \Delta x/N)(1-R)} = F_+(x)R\exp(-\mu_a \Delta x/N) \times$$
$$\times \frac{1-\exp(-2\mu_a \Delta x)(1-R)^N}{1-\exp(-2\mu_a \Delta x/N)(1-R)}. \tag{16}$$

Finding the limit of the ratio of 'increment' of $F_-(x)$ on the segment Δx to Δx at $\Delta x \to 0$, we obtain a differential equation for $F_-(x)$ [14]:

$$\frac{dF_-(x)}{dx} = \mu_a F_-(x) - \beta_2^+ F_+(x), \tag{17}$$

where

$$\beta_2^+ = (2\mu_a + \mu_s)\frac{R\exp(-\mu_a/\mu_\rho)}{1-\exp[-(2\mu_a+\mu_s)/\mu_\rho]} \tag{18}$$

is the backscattering coefficient for the flux $F_+(x)$. We can see that $\beta_2^+ \neq \mu_s$.

Thus, the system of differential equations solved in the SS approximation for a medium with continuous absorption and discrete scattering will have the form

$$\begin{aligned} \frac{dF_+(x)}{dx} &= -\beta_1^+ F_+(x), \\ \frac{dF_-(x)}{dx} &= \mu_a F_-(x) - \beta_2^+ F_+(x), \end{aligned} \tag{19}$$

where for the attenuation coefficient of flow $F_+(x)$ the notation

$$\beta_1^+ = \mu_a + \mu_s \tag{20}$$

is introduced.

In spite of all the external similarity, system (19) is fundamentally different from system (1), since in a general case $\beta_2^+ < \mu_s$. Only for $\mu_a = 0$ (i.e., in the limit $\mu_a \to 0$) $\beta_2^+ = \mu_s$, which means that not all scattered photons of the flux $F_+(x)$ are converted by the segment Δx into photons of the flux $F_-(x)$. Some of them are lost due to absorption immediately within the segment Δx. Thus, in the presence of discrete scatterers inside a continuous absorbing medium at $\mu_a \neq 0$ values of $F_-(x)$ will differ from those obtained using Eqn (4).

Under the same boundary conditions as indicated in Section 3.1, system (19) has solutions

$$F_+(x) = F_0 \exp(-\beta_1^+ x), \tag{21}$$

$$F_-(x) = F_0 \frac{\beta_2^+}{2\mu_a + \mu_s}\exp(-\beta_1^+ x). \tag{22}$$

A numerical comparison of these solutions and the solutions given in Section 3.1 is shown in Fig. 4 for the same values of μ_a and μ_s as in Fig. 2. It can be seen that the values of the fluxes $F_+(x)$ in these two cases do not differ, since the value of β_1^+ remains unchanged. However, the difference in the fluxes $F_-(x)$ near the outer boundary of the medium is clearly manifested.

Obviously, the numerical calculation by the MC method with classical probabilistic parameters for a medium with continuous scattering in this case of discrete scatterers will also give the value of $F_-(x)$, which differs from the exact solution (22), like the analytical solution in Section 3.1. Then the question of how the probabilistic parameters of the MC algorithm should be changed in order to numerically obtain a

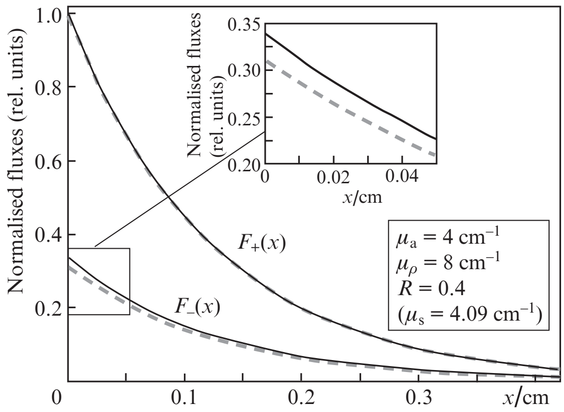

Figure 4. Analytical solutions of 1D problems in the SS approximation for a medium with continuous absorption and continuous scattering (solid curves) and a medium with continuous absorption and discrete scattering (dashed curves). The values of the fluxes $F_+(x)$ and $F_-(x)$ are normalised to F_0.

result corresponding to (22) is legitimate. We dare to suggest an easy way.

According to Eqn (21), the function

$$B_+(x') = 1 - \exp(-\beta_1^+ x') \tag{23}$$

determines the fraction of photons 'lost' by the flux $F_+(x)$ due to scattering and absorption along the path segment $[0; x']$: $0 \leqslant B_+(x') \leqslant 1$. When proceeding to the probabilistic model, it is replaced by the probability distribution function $D_{l_+}(x')$ of the random variable l_+ that simulates it:

$$B_+(x') = D_{l_+}(x') \equiv P\{l_+ \leqslant x'\}, \tag{24}$$

determining the probability that $l_+ \leqslant x'$, and also defined in the interval [0; 1]. Further, according to the inverse transformation method, to find the random variable l_+ with a given distribution $D_{l_+}(x')$, we can take a random variable ξ_1 uniformly distributed on the interval [0; 1], find the inverse function $D_{l_+}^{-1}(\xi_1)$ and use it to calculate l_+ [7, 18]. The resulting random variable l_+ will have the distribution $D_{l_+}(x')$. Randomly generating different ξ_1 and taking into account that the random variables $1-\xi_1$ and ξ_1 have the same uniform distribution on the segment [0; 1], symmetric with respect to the value $\xi_1 = 0.5$, we obtain the required set of l_+ when generating ξ_1:

$$l_+ = D_{l_+}^{-1}(\xi_1) = -\frac{\ln\xi_1}{\beta_1^+} = -\frac{\ln\xi_1}{\mu_a + \mu_s}. \tag{25}$$

Here l_+ coincides with l_+^{cl} (6).

For the photon flux $F_-(x)$ in the SS approximation

$$B_-(x') = 1 - \exp(-\mu_a x'). \tag{26}$$

By analogy with l_+, in this case we arrive at the expression

$$l_- = -\frac{\ln\xi_2}{\mu_a}. \tag{27}$$

Based on the empirical (frequency) definition of the probability as the frequency of desired event occurrence against the background of all possible events, the probability of scattering P_s on any infinitely small segment Δx inside the medium should be determined by the fraction of scattered $F_+(x)$ photons, which form the $F_-(x)$ flux, against the background of all photons lost by the flux $F_+(x)$. This fraction is determined when deriving the system of equations (19) and is equal to $\beta_2^+ F_+(x)\Delta x$. In this case, the complete set of events are all photons lost by the flux $F_+(x)$ on the segment Δx, i.e., the value of $\beta_1^+ F_+(x)\Delta x$. The ratio of these quantities will be exactly the required scattering probability P_s:

$$P_s = \frac{\beta_2^+}{\beta_1^+}. \tag{28}$$

Thus, the complete set of probabilistic parameters of the MC method in the SS approximation for a 1D problem with discrete scatterers should look as follows:

$$l_+ = -\frac{\ln\xi_1}{\beta_1^+}, \quad P_s = \frac{\beta_2^+}{\beta_1^+}, \quad l_- = -\frac{\ln\xi_2}{\mu_a}. \tag{29}$$

Comparing Eqn (29) with Eqns (5)–(7), one can notice that the probabilities P_s^{cl} and P_s are different, since in the general case $\beta_2^+ \neq \mu_s$. As shown in Fig. 5, the solution by the MC method with probabilistic parameters (29) ideally coincides with the analytical solution (22) for the flow $F_-(x)$, while the classical MC method gives a solution with a systematic error due to the fact that $P_s^{\text{cl}} \neq P_s$. In short, the use of the SS albedo for calculating the scattering probability P_s in this problem is no longer correct.

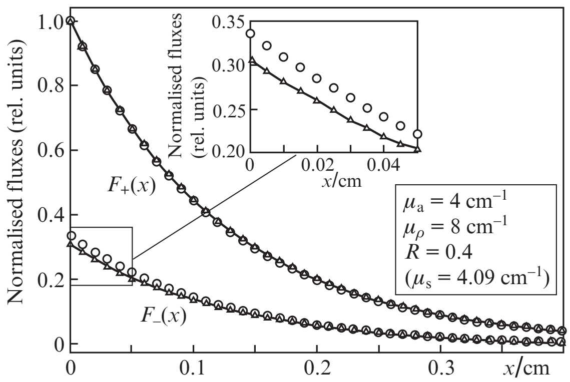

Figure 5. Analytical solutions (solid curves) and numerical solutions by the MC method with different probabilistic parameters of the 1D problem in the SS approximation for a medium with discrete scattering (triangles) and a medium with continuous absorption and continuous scattering (circles). The values of the fluxes $F_+(x)$ and $F_-(x)$ are normalised to F_0.

4. Model problem for multiple scattering

The problem of multiple scattering inside a 1D medium with continuous absorption and discrete scattering is also quite indicative. Although we have previously reported on the results obtained for it [12], it is interesting to present the solution of this problem and give its comparative analysis with the numerical solution by the MC method in order to formulate substantiated conclusions drawn from the results of the study. For multiple scattering in a medium with continuous absorption and discrete scattering, the system of modified Kubelka–Munk equations [11, 14]

$$\frac{dF_+(x)}{dx} = -\beta_1 F_+(x) + \beta_2 F_-(x),$$
$$\frac{dF_-(x)}{dx} = \beta_1 F_-(x) - \beta_2 F_+(x) \quad (30)$$

should be solved, where

$$\beta_1 = \omega \times \frac{\mu_a - \mu_\rho \ln(1-R) + \mu_\rho \ln\left[1 - \omega + \sqrt{\omega^2 - R^2 \exp(-2\mu_a/\mu_\rho)}\right]}{\sqrt{\omega^2 - R^2\exp(-2\mu_a/\mu_\rho)}}; \quad (31)$$

$$\beta_2 = R\exp(-\mu_a/\mu_\rho) \times \frac{\mu_a - \mu_\rho \ln(1-R) + \mu_\rho \ln\left[1 - \omega + \sqrt{\omega^2 - R^2 \exp(-2\mu_a/\mu_\rho)}\right]}{\sqrt{\omega^2 - R^2\exp(-2\mu_a/\mu_\rho)}}; \quad (32)$$

$$\omega = \frac{1 - (1-2R)\exp(-\mu_a/\mu_\rho)}{2}. \quad (33)$$

Here not only $\beta_2 \neq \mu_s$, but also $\beta_1 \neq \mu_a + \mu_s$. The solution of system (30) is known and has the form [5]

$$F_+(x) = C_1\exp(-\alpha x) + C_2\exp(\alpha x),$$
$$F_-(x) = C_1 A_- \exp(-\alpha x) + C_2 A_+ \exp(\alpha x), \quad (34)$$

where C_1 and C_2 are the integration constants determined from the boundary conditions (see Section 3.1);

$$\alpha = \sqrt{\beta_1^2 - \beta_2^2}; \quad A_+ = \frac{\beta_2}{\beta_1 - \alpha}; \quad A_- = \frac{1}{A_+}.$$

Since the multiple scattering regime is realised in the medium, the photons are equally scattered and absorbed along the path of their propagation both in the flux $F_+(x)$ and in the flux $F_-(x)$. Therefore, in the numerical simulation by the MC method, the use of a single photon mean free path

$$l = -\frac{\ln\xi}{\beta_1} \quad (35)$$

is justified.

As shown in Ref. [12], taking into account (35), the correspondence of the analytical results to the numerical results of the MC simulation both for the flux $F_+(x)$ and for the flux $F_-(x)$ is achieved when the scattering probability is specified in a form similar to (28):

$$P_s = \frac{\beta_2}{\beta_1}. \quad (36)$$

The results of comparing the analytical solution (34) with allowance for (31) and (32) and the numerical solution by the MC method with different probabilistic parameters for multiple scattering are presented in Fig. 6. In this case, parameters (35) and (36) with $\beta_1 = \mu_a + \mu_s$ and $\beta_2 = \mu_s$ were used as classical probabilistic parameters in the MC algorithm. The discrepancy in the results for fluxes is seen to reach 10% at the boundary of the medium. It is important that in the case of multiple scattering, the discrepancy between the results of the classical simulation by the MC method and the exact analytical results (34) is observed even for the flux $F_+(x)$. To eliminate this discrepancy, it is necessary to use the correct probabilistic parameters β_1 (31) and β_2 (32).

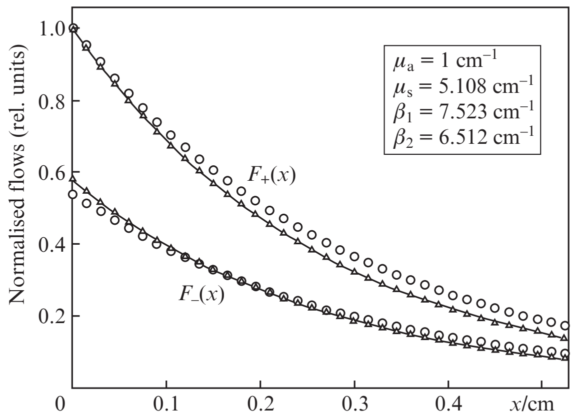

Figure 6. Analytical solutions (solid curves) and numerical solutions by the MC method with different probabilistic parameters of the 1D problem with multiple scattering for a medium with discrete scattering (triangles) and a medium with continuous absorption and continuous scattering (circles). The values of the fluxes $F_+(x)$ and $F_-(x)$ are normalised to F_0.

5. Conclusions

We analysed the applicability of the probabilistic parameters of the numerical MC algorithm generally accepted in biomedical optics for problems of light transfer in turbid media with continuous absorption and discrete scattering. For this purpose, we obtained exact analytical solutions of model 1D problems for such media and compared them with the results of numerical modelling by the MC method. Comparison has shown that the use of generally accepted (classical) probabilistic parameters of the MC algorithm causes a systematic numerical error for the considered turbid media, which is not eliminated by increasing the number of played photons. Additionally, we substantiated the necessary refined probabilistic parameters for numerical simulation by the MC method in the case of media with discrete scattering and showed that their application leads to perfect coincidence of numerical and analytical results. Thus, one of the main conclusions formulated from the results of the study is the conclusion that it is necessary for each specific problem to choose reasonable values of the probabilistic parameters of the MC algorithm, which may differ from the generally accepted ones.

Another important conclusion is that the choice of adequate probabilistic parameters based on a priori phenomenological concepts is most likely impossible. It is hardly possible to guess the form of Eqns (31) and (32). Consequently, for a competent substantiation of the probabilistic parameters, it is necessary to have an exact form of expressions for the coefficients of the original equations, which can be obtained only analytically based on ideas about the internal structure of the medium, as was done, for example, for β_2^+ (18). Strictly speaking [see the remark after Eqn (6)], all classical probabilistic parameters are also based on well-known analytical solutions, for example, on expression (2), in which the coefficients of system (1) are given *a priori*. The MC method allows only finding a numerical solution of the system of initial equations in the form in which they are formulated. If the original system is formulated with incorrect coefficients, then its solution by the MC method will also be erroneous, and vice versa. It is another matter that the discrepancies in the results obtained in this work when using the classical probabilistic parameters of the MC algorithm are so far not very large for 1D problems, about 10% or less. If they do not increase in 2D and 3D problems, which requires additional investigation, this may be sufficient for many practical problems, for which an analytical solution is unknown. In particular, when searching for an unknown analytical solution and unknown exact expressions for the coefficients of the initial equations of any problem in TT, the classical version of the MC method immediately gives a certain reference point when solving with an accuracy of no worse than 90% (according to our data), and this is its undoubted plus.

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