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Determination of the optical properties of turbid media from a single Monte Carlo simulation

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Abstract. We describe a fast, accurate method for determination of the optical coefficients of 'semi-infinite' and 'infinite' turbid media. For the particular case of time-resolved reflectance from a biological medium, we show that a single Monte Carlo simulation can be used to fit the data and to derive the absorption and reduced scattering coefficients. Tests with independent Monte Carlo simulations showed that the errors in the deduced absorption and reduced scattering coefficients are smaller than 1% and 2%, respectively.

Knowledge of the optical properties of biological tissue is important for many applications of light in medicine. Derivation of the absorption and scattering coefficients from a set of measurements requires a theoretical model. The transport equation (Ishimaru 1978) can be used to describe light propagation in tissue, but because this equation can only be solved numerically for most cases of interest, the diffusion approximation (Ishimaru 1978, Patterson *et al* 1991) is often applied. Solutions of the diffusion equation for simple geometries can be readily obtained (Patterson *et al* 1989, Moulton 1990, Haskell *et al* 1994) but the diffusion approximation breaks down near a radiation source (Kienle *et al* 1996, Hielscher *et al* 1995). This region is of special interest in applications such as endoscopy and coherent light measurements.

The Monte Carlo method (Wang *et al* 1995) is often used to solve the transport equation numerically, but it is too slow to use in an iterative algorithm where the optical properties are estimated by comparison of simulation results with actual measurements. Here we show that this limitation can be overcome by using a single Monte Carlo simulation if the refractive index and the anisotropy factor of the medium are known. This is possible because a Monte Carlo simulation for a certain anisotropy factor, g, refractive index, n, and scattering coefficient, μ_s, can be used to calculate the desired quantities for all possible absorption cofficients, μ_a, by applying Beer's law. Also, the results for all scattering coefficients (if g and n are constant) can be obtained by suitably scaling the outcome of a single Monte Carlo simulation, because different μ_s values change only the distances between the interaction points on the photon paths through the tissue. This 'Mono Monte Carlo' approach can be used for steady state and for time-resolved problems if the geometry is infinite or semi-infinite. In this study we illustrate the concept by estimating the reduced scattering coefficient, $\mu_s' = \mu_s(1-g)$, and the absorption coefficient from the time-resolved diffuse reflectance from a semi-infinite turbid medium.

In the Monte Carlo simulations a point source with an infinitely small pulse was used and the length of the photon path was computed to obtain the travel time through the turbid medium. Convolution can be applied to calculate the reflectance for arbitrary sources. As

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phase-function the Henyey-Greenstein function (Henyey and Greenstein 1941) was used. (We simulated a slab with a thickness of 30 m. Thus, the probability that a photon reached the lower boundary equaled zero and the geometry could be considered as semi-infinite.)

First we demonstrate that different anisotropy factors do not significantly influence the time-resolved reflectance if g is close to 1, as is the case for tissue, so that the results of a single simulation can be used. In general the solution to the transport equation depends on four different optical parameters n, g, μ_s and μ_a. The refractive index, n, is about 1.4 for all soft tissue (Bolin *et al* 1989). The number of unknown optical coefficients can be further reduced if the principle of similarity is valid. This principle states that different combinations of g and μ_s yield similar results for dependent quantities such as diffuse reflectance. The simplest relationship is that conservation of $(1-g)\mu_s$ will ensure similarity. We performed Monte Carlo simulations of time-resolved reflectance, $R(t)$, for different optical parameters and radial distances, ρ, from the source to investigate the validity of this relationship. Figure 1 shows $R(t)$ for $\mu_s' = 1$ mm^{-1} and $\mu_a = 0$ mm^{-1} at $\rho = 2.25$, 3.25 and 4.75 mm for $g = 0$, 0.5, 0.8 and 0.9. This figure, and calculations with other sets of optical coefficients, shows that the simple similarity relation is valid for $g \geqslant 0.8$. Because the anisotropy factor of tissue is normally greater than 0.8 (Cheong *et al* 1990) and Monte Carlo calculations are faster for smaller g, $g = 0.8$ was applied in the Monte Carlo simulations in this study.

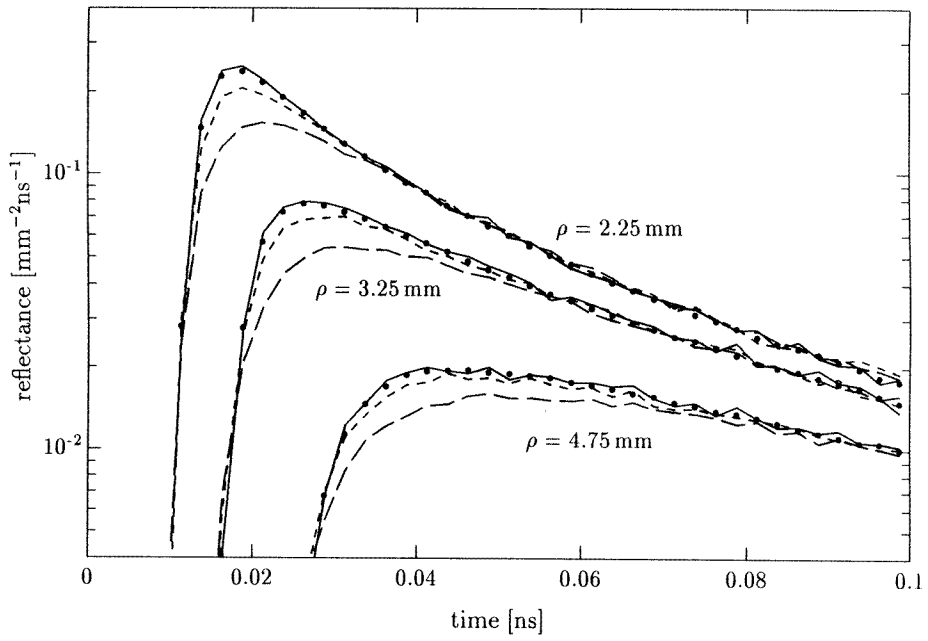

Figure 1. Time-resolved diffuse reflectance for different anisotropy factors, $g = 0$ (long dashed curve), $g = 0.5$ (dashed), $g = 0.8$ (circles) and $g = 0.9$ (solid), at distances $\rho = 2.25$, 3.25 and 4.75 mm. The other optical properties are $\mu_s' = 1$ mm^{-1}, $\mu_a = 0$ mm^{-1} and $n = 1.4$.

Determination of the optical properties of a semi-infinite or infinite turbid medium with a single Monte Carlo simulation is based on the following principle: it is possible to extract from the output of one simulation, performed with certain optical parameters, the desired quantities for other optical coefficients if the anisotropy factor is the same (or the similarity

relation is valid) and the refractive index does not change. From the results of a Monte Carlo simulation performed with certain reference parameters, μ_{sr} and μ_{ar}, the desired quantity, such as the diffuse reflectance, can be obtained for μ_{sr} and any absorption coefficient μ_a using Beer's law. For example, if $\mu_{ar} = 0$, the time-resolved diffuse reflectance, $R(\rho, t)$, can be calculated for any μ_a from the reference time-resolved reflectance $R_r(\rho, t)$ by

$$R(\rho, t) = R_r(\rho, t) \exp(-\mu_a c\, t) \tag{1}$$

where c is the speed of light in the turbid medium. For the case $\mu_{ar} = 0$, the results of the single Monte Carlo simulation can also be scaled to yield the desired quantities for any scattering coefficient. This is because altering the scattering coefficient in the simulation results only in different lengths of the photon paths through the tissue (Graaff *et al* 1993). In the case of time-resolved reflectance this means that $R(\rho, t)$, for arbitrary μ_s and $\mu_a = 0$, can be derived from $R_r(\rho, t)$ calculated for μ_{sr} and $\mu_{ar} = 0$ using

$$R(\rho, t) = \left(\frac{\mu_s}{\mu_{sr}}\right)^3 R_r\left(\rho\frac{\mu_s}{\mu_{sr}}, t\frac{\mu_s}{\mu_{sr}}\right). \tag{2}$$

The scaling factor for the distance variable is due to the different path lengths of the photons, and consequently the time variable has to be scaled by the same value. A factor $(\mu_s/\mu_{sr})^2$ (before R_r) stems from the scaling of the area and the remaining factor (μ_s/μ_{sr}) from the scaling of the time.

In principle, using equation (1) and equation (2), $R(\rho, t)$ can be easily and quickly calculated for any absorption and scattering coefficients. However, it is not possible to calculate $R_r(\rho, t)$ with Monte Carlo simulations for continuous ρ and t values, but only for certain distance and time intervals, $R_r(\rho_i, t_i)$, centered at ρ_i and t_i. As a consequence, the results of the reference Monte Carlo simulation have to be interpolated to compute $R(\rho, t)$ with equation (2). In this study a Monte Carlo simulation for $\mu_s' = 1$ mm^{-1}, $g = 0.8$ and $\mu_a = 0$ mm^{-1} was performed, and $R_r(\rho_i, t_i)$ was recorded for distances between $\rho_1 = 0.25$ mm and $\rho_{40} = 19.75$ mm at intervals of 0.5 mm, and for times between $t_1 = 1.25$ ps and $t_{40} = 98.75$ ps at intervals of 2.5 ps, and between $t_{41} = 105$ ps and $t_{230} = 1995$ ps at intervals of 10 ps. 33 million photon histories were used to achieve good statistics. A non-linear regression method was applied to estimate the optical coefficients from time-resolved reflectance data using the Mono Monte Carlo approach. Because it is difficult in practice to make absolute measurements of the time-resolved reflectance, we fitted relative data. Thus, not only μ_a and μ_s' but also a scaling parameter was fitted. For the non-linear regression, reflectance data up to $t = 1$ ns were used, and the logarithm of $R(t)$ was fitted. This requires that $\mu_s' < 2$ mm^{-1}, because of the scaling of equation (2) and because the maximum time recorded in the Monte Carlo simulation was 2 ns. In the ρ direction the logarithm of $R_r(\rho_i, t_i)$ was linearly interpolated. For example, if the ρ-scaling of equation (2) results in $\rho' = \rho\mu_s/\mu_{sr}$ with $\rho_k < \rho' < \rho_{k+1}$, then the time-resolved reflectance, $R(\rho', t_i)$, is calculated from

$$R(\rho', t_i) = \exp\left[(1-h)\ln(R_r(\rho_k, t_i)) + h\ln(R_r(\rho_{k+1}, t_i))\right] \tag{3}$$

where

$$h = \frac{\rho' - \rho_k}{\rho_{k+1} - \rho_k}. \tag{4}$$

Usually the time-resolved reflectance is measured at a certain distance, ρ, at different time-values $R(t_i)$. Thus, for each iteration of the non-linear regression the reflectance must be evaluated at these times requiring interpolation of the reflectance data produced by the Mono Monte Carlo. Initially we used a linear interpolation of $\ln(R(t_i))$ between

the adjacent time values, but this resulted in optical coefficients which were in many cases incorrect and which depended on the initial estimates for the non-linear regression. Linear interpolation failed because of statistical noise in the Monte Carlo data and rapid changes in the reflectance at short times and small distances. Algorithms such as polynomial interpolation or cubic spline interpolation provided only marginal improvement. In order to improve the interpolation in time we sought an arbitrary function to approximate the $R(t)$ curves of the Monte Carlo simulation. Equation (5) provided a good fit to the logarithm of the time-resolved reflectance for all ρ values:

$$\ln(R(t)) = c_0 + c_1 \ln t + c_2(\ln t)^2 ... + c_{10}(\ln t)^{10} . \tag{5}$$

The time-resolved reflectance data for all 40 distances were fitted to equation (5) and the fitting parameters, c_0, ..., c_{10} at each distance were stored for later application.

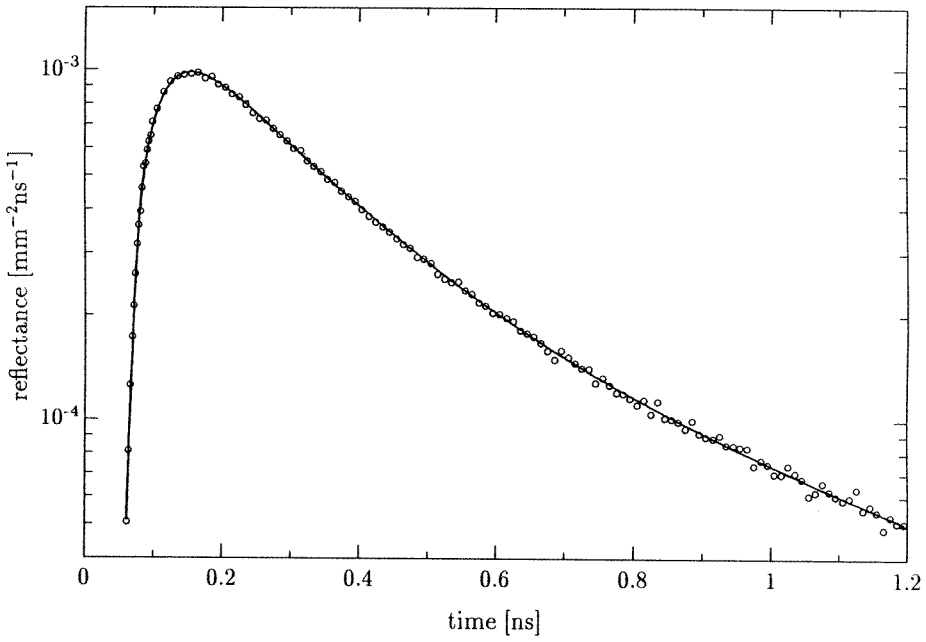

Figure 2. Regression (solid curve) to a Monte Carlo simulation (circles) using equation (5). The parameters of the simulation are $\mu_s' = 1$ mm^{-1}, $\mu_a = 0$ mm^{-1}, $n = 1.4$, $g = 0.8$ and $\rho = 9.75$ mm.

Figure 2 shows one comparison of the Monte Carlo data and the fit generated from equation (5). Using these fitting functions the interpolation errors in the time axis could be minimized and the noisier data at large time values could be smoothed. Accordingly, the non-linear regression performance was greatly improved and delivered the right optical coefficients in most cases when tested with independent Monte Carlo simulations. However, for small distances and small reduced scattering coefficients the derived optical coefficients were still incorrect. This was caused by the larger interpolation errors in the ρ variable (equation (3)) at small $\rho\mu_s'$, where the second derivative at the maximum value of $R(t)$ and the first derivative at early times are greater. We solved this problem by creating $R(t)$ curves for intermediate distances by fitting $\ln(R_r(\rho_i, t_i))$ for constant t_i values between $t_1 = 1.25$ ps and $t_{29} = 73.75$ ps to an eighth order polynomial. Between each two adjacent

$R(\rho_i, t = \text{constant})$ data points in the above mentioned time region, three new values were deduced from the fitting curves, increasing the number of $R(\rho = \text{constant}, t)$ curves from 40 to 157. These 157 curves were then fitted to equation (5) and a subset is shown in Figure 3. (In Figure 3 the reflectance for small distances exceeds 1 $\text{mm}^{-2}\text{ns}^{-1}$ in a certain time region. To calculate the probability that an incident photon is re-emitted the reflectance has to be integrated over a certain time interval and area. Thus, the probability does not exceed unity.)

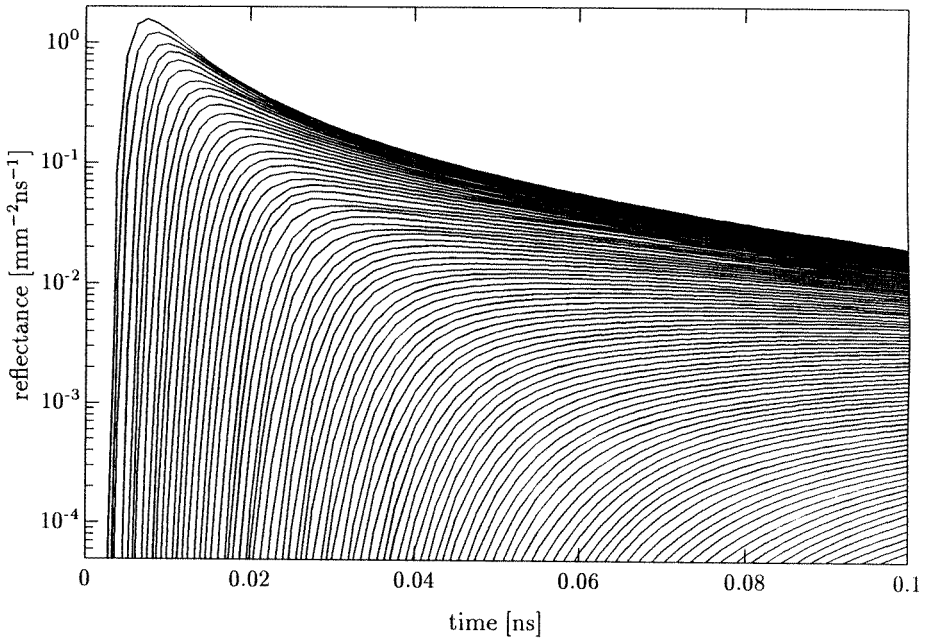

Figure 3. A sample of the 157 fitted time-resolved reflectance curves using equation (5). The parameters of the Monte Carlo simulations are $\mu_s' = 1.0$ mm^{-1}, $\mu_a = 0$ mm^{-1}, $g = 0.8$, $n = 1.4$ and $1 < \rho < 12.5$ mm; the top curve is for $\rho = 1$ mm, the bottom curve is for $\rho = 12.5$ mm, and the other curves have been calculated for intervals of 0.125 mm.

The performance of the non-linear regression using these fitted curves was excellent even for smaller ρ and μ_s' values. Independent Monte Carlo simulations with $\mu_s' = 0.5$ mm^{-1}, 0.72 mm^{-1}, 1.0 mm^{-1} and 1.5 mm^{-1} were performed for the same time values as in the reference simulation to test the non-linear regression. 120 reflectance curves for distances $2.5/\mu_s' < \rho < 20$ mm ($\rho\mu_s' < 20$) and an absorption coefficient of $\mu_a = 0.02$ mm^{-1} were used. The mean error in the derived optical parameters was smaller than 2% for the reduced scattering coefficient and smaller than 1% for the absorption coefficient. The reflectance values at the earliest times (where the reflectance was less than 10% of the peak reflectance) were not included, but enough data before the maximum of the curve were used so that no essential information was lost. The absolute error in the absorption coefficient was found to be independent of the value of the absorption coefficient, resulting in a greater relative error for smaller μ_a values.

In conclusion, a new method was developed to derive the reduced scattering and absorption coefficients of semi-infinite and infinite turbid media. Using the example of time-

resolved reflectance from a semi-infinite medium, we showed that the reduced scattering coefficient and the absorption coefficient could be determined with errors smaller than 2% and 1%, respectively. The performance of the method was good even close to the source ($\rho = 2.5/\mu_s'$) and, in addition, it can be applied for very large absorption coefficients. (Thus, the method works for the diffuse and the non-diffuse limit of photon propagation.) Either of these conditions can invalidate algorithms based on approximate solutions to the transport equation, such as diffusion theory. However, one has to pay particular attention to potential interpolation errors in the scaling of the reference Monte Carlo data. Once the reference simulation has been performed and the parameters of the regressions of the time-resolved data to equation (5) have been stored, the optical coefficients can be determined from time-resolved reflectance data in approximately one second with a state-of-the-art personal computer. We note that if the Mono Monte Carlo method is used to determine the optical coefficients from steady-state reflectance from a semi-infinite medium (Kienle *et al* 1996), the interpolation problem is less important because the reflectance curves are smoother and monotonically decreasing with distance.

For the simulations an anisotropy factor of $g = 0.8$ and a refractive index of $n = 1.4$ were used. We showed that the similarity relation is valid for the high g values found in tissue enabling the use of one anisotropy factor. In order to investigate the influence of a different value of n on the performance of the Mono Monte Carlo method, we performed simulations with $n = 1.35$ and determined the optical properties using $n = 1.4$ in the reference simulation. The absorption coefficient could be estimated within 3%, but the error in the reduced scattering coefficient was usually much greater, exceeding 10% for $\rho < 10$ mm. Therefore, knowledge of the tissue refractive index improves the accuracy of the μ_a and μ_s' estimates.

The Mono Monte Carlo method can also be applied in the frequency domain by numerical Fourier transformation of the time-resolved reflectance data at each evaluation of $R(t)$ in the non-linear regression.

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