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Estimation of scattering volume in short distance reflectance measurements by Monte Carlo modelling

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The depth of light penetration is an interesting issue in various tissue optics experiments. The measurements of remitted light distribution was shown to allow for estimation of optical properties. However, in case of measurements with a short distance between the emitter and the detector, the diffusion equation fails, and the proposed methods cannot be applied. The aim of this study was to develop a simple method for estimation of the light penetration depth for short-distance measurements of remitted light. The idea is based on the analysis of the diffusely back-scattered light distribution adjacent to the emitter for the assessment of the scattering volume. The Monte Carlo method was used for theoretical estimation of the relationship between the light distribution around emitting fiber and the depth of light scattering volume. Two series of Monte Carlo simulations were performed: the first one with limited and the second one with unlimited scattering volume. In both series the values of absorption and scattering coefficients were altered within ranges typical of human tissues. The results of this study show that: the diffuse reflectance is strongly dependent on the absorption and scattering properties of the tissue and it is possible to estimate the depth of the scattering volume by use of the short distance profile of diffusely back-scattered light as measured at the surface of the tissue.

1. Introduction

The depth of the light penetration is an interesting issue in various tissue optics experiments. It was shown that measurement of remitted light distribution allows for estimation of optical properties. However, in case of measurements with a short distance between the emitter and the detector, the diffusion equation fails, and the proposed methods cannot be applied. A short emitter–detector distance is applied in measurements of remitted light distribution in endoscopic tissue monitoring, short distance near infrared spectroscopy as well as in laser-Doppler flowmetry. In these applications, the lack of measurement volume estimate limits their clinical useful-

ness. These limitations could be overcome, if the optical properties of the living tissue such as absorption, scattering and anisotropy coefficients were known.

The *in vivo* experimental estimation of tissue optical properties, however, is cumbersome, and the equipment necessary for the phase shift detection as well as for the time of flight measurements is still expensive [1]–[3]. None of these methods can therefore be used in routine *in vivo* biomedical applications. The *in vitro* estimation of tissue optical properties is possible with the application of integrating spheres [4]–[6], but it is known that the physical and chemical properties of the tissue (and, consequently, the optical properties) change when the tissue sample is isolated from the living organism. *In vitro* studies can therefore give only a raw estimation of the optical properties of the living tissue. Some studies have demonstrated that the analysis of the diffusely back-scattered light distribution profile can be also applied for estimation of the optical properties of the tissue [7]–[12]. The latter approach forms the basis of the methods for assessment of the scattering volume further developed in this paper.

Many theoretical methods have been used up to now for evaluation of the light distribution in the tissue [13]–[15]. Unfortunately, the diffusion theory cannot be used for short distance measurements in which the measurement volume of the tissue is relatively small (below 1 mm^3). The mean path-length of the photon flight between successive interactions within the tissue is within the same range as the distance over which the distribution profile is to be estimated. Therefore, in this work, the Monte Carlo simulation method [14] was used for estimation of the distribution profile and scattering volume.

The aim of the present study was to assess the distribution of the diffusely back-scattered light from the tissue with the use of the Monte Carlo simulation method and to develop a simple algorithm for estimation of the light penetration depth.

2. Methods

Monte Carlo modelling was used to study the diffusely back-scattered light distribution around the emitter location and to evaluate the relation between this distribution and the depth of light penetration into the tissue. The distribution profile was parameterized by the use of a modified function proposed by Groenhuis [7], [8]. A factor describing the depth of the scattering volume, that correlates well with the light distribution profile parameters, is proposed.

The Monte Carlo modelling software written in the standard C language developed by Jacques and Wang from the University of Texas was used [16], [17] for the calculations. The program was recompiled on an IBM-PC class computer working under control of the Linux system.

Two series of Monte Carlo simulations were carried out. First, a semi-infinite homogenous tissue model was used as shown in Fig. 1. The thickness of the tissue layer was set to be large (d_{max}= 10 cm) in order to capture the whole laser light

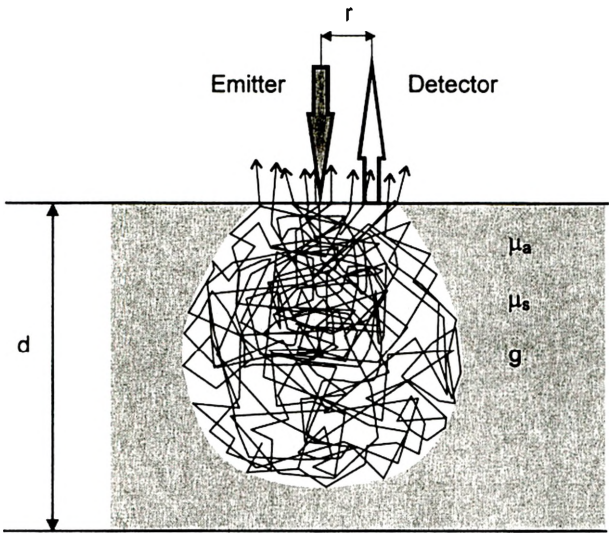

Fig. 1. Semi-infinite model used in the first set of Monte Carlo simulations (μ_a – absorption coefficient, μ_s – scattering coefficient, g – anisotropy factor).

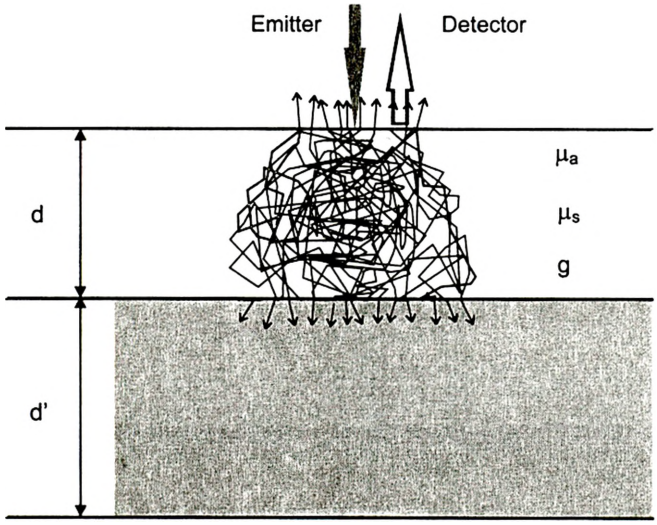

Fig. 2. Two-layer model used in the second set of Monte Carlo simulations.

scattering volume. The refractive indices for all the layers were 1.33, to avoid the influence from reflection and refraction at the interfaces. The relationship between the diffuse reflectance and the emitter-detector distance was estimated from these simulations. The following function proposed by GROENHIUS [7], [8] and modified by FARRELL [9] was fitted to the data obtained in the simulations

$$R_d(r) = \frac{c_1}{r^m} \exp(-c_2^2 r^2) \tag{1}$$

where $R_d(r)$ is the relative amount of the diffusely back-scattered light at the distance r from the emitter, and m, c_1 and c_2 are the function parameters to be fitted.

Second, a two-layered tissue model as shown in Fig. 2 was used. Simulations with different thicknesses of the first layer were performed. The deeper layer in this model was semi-infinite and totally light absorbing. The diffuse reflectance coefficient defined as the number of remitted photons normalized by the total number of emitted photons was calculated for different thicknesses of the first layer. In this relation the inclination point was observed where the rate of the back-scattered light intensity changes was the biggest. Then, the first derivative $r_d(d)$ of this function describing the probability density of photons travelling between the emitter and the photodetector was calculated. The Lorentz distribution was fitted to $r_d(d)$ according to the following equation:

$$r_d(d) = \frac{\mathrm{d}R}{\mathrm{d}d} = r_{d0} + \frac{2A}{\pi}\left(\frac{\omega}{4(d-d_0)^2+\omega^2}\right) \tag{2}$$

where r_{d0} is the baseline offset, A is the total area under the curve from the baseline, d_0 is the center of the peak and ω the width of the peak at half height. It is expected that the thickness d_0 for which the $r_d(d)$ function has maximum, correlates with the depth of the scattering volume.

In both series of simulations, the absorption μ_a and scattering μ_s coefficients varied in ranges typical of human tissues [15]. The absorption coefficient was changed from $\mu_a = 0.2$ cm^{-1} to $\mu_a = 9.2$ cm^{-1} in steps of 1 cm^{-1}. The scattering coefficient was changed from $\mu_s = 100$ cm^{-1} to 550 cm^{-1} in steps of 50 cm^{-1}. All simulations were performed with a constant value of the anisotropy factor $g = 0.9$. The laser source was simulated as a Gaussian beam with a wavelength of $\lambda =$ 780 nm, a half-width diameter of 250 μm and a power of 1 mW. All simulations were carried out for the set of $5 \cdot 10^5$ photons.

Functions (1) and (2) were fitted to the results of the simulations by the Levenberg–Marquardt iterations, and finally, the function parameters d_0, c_1, c_2 were obtained for all μ_a and μ_s values. The non-linear fitting function implemented in Origin v. 4.1 was used.

3. Results

The results obtained from the first series of simulations are presented in Figs. 3 and 4. In Figure 3 the relation between the diffuse reflectance and the emitter –detector distance for different scattering coefficients and constant absorption coefficient ($\mu_a = 3.2$ cm^{-1}) is demonstrated. Similar relations for a constant scattering coefficient ($\mu_s = 300$ cm^{-1}) and various absorption coefficients are presented in Fig. 4. The diffuse reflectance increases and extends further out from the source when the scattering is increased or absorption is decreased.

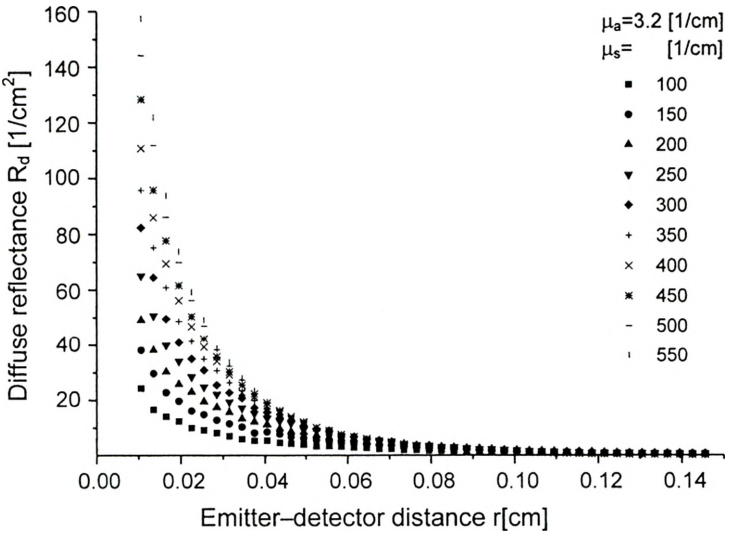

Fig. 3. Diffuse reflectance *vs.* emitter–detector distance for different scattering coefficients ($\mu_s = 100 - 550$ cm^{-1}) and constant absorption coefficient ($\mu_a = 3.2$ cm^{-1}).

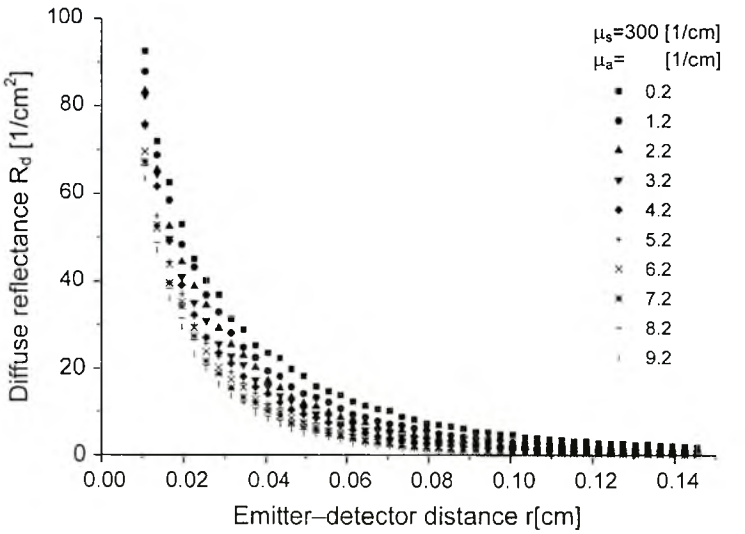

Fig. 4. The same as in Fig. 3, but for constant scattering coefficient ($\mu_s = 300$ cm^{-1}) and various absorption coefficients ($\mu_a = 0.2 - 9.2$ cm^{-1}).

Typical diffusely back-scattered light distribution profiles obtained for selected values of coefficients μ_s and μ_a are presented in Fig. 5. The fitted function (1) is also shown here. After fitting this function to many different diffusely back-scattered light distribution profiles, we found that the value of $m = 0.6$ gave the lowest fitting errors

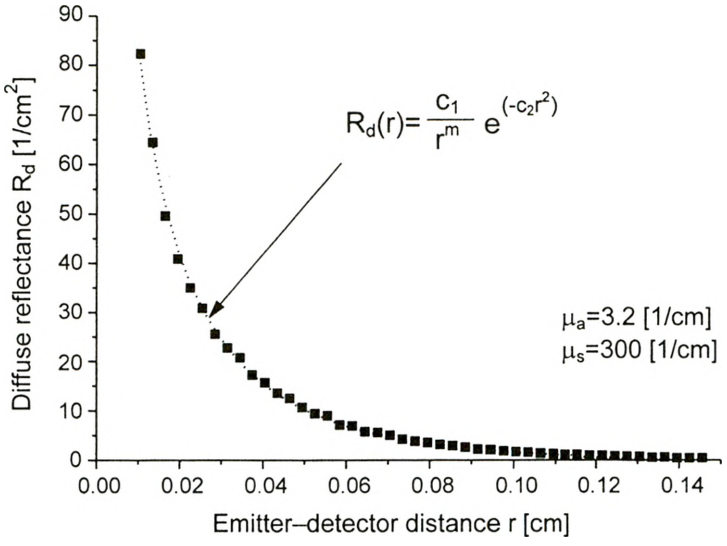

Fig. 5. Typical profile of a diffusely back-scattered light distribution ($\mu_a = 3.2$ cm^{-1}, $\mu_s = 300$ cm^{-1}, $g = 0.9$) and the Groenhuis–Farrell function fitted to the results of simulations.

for the range of emitter–detector distance $r = 0 - 1.5$ mm. The fitting error was in the range between 5% and 30%.

The parameters of the Groenhuis–Farrell functions (1) fitted to the results obtained in this series of simulations were correlated with optical properties of the tissue model. In Figures 6 and 7, the 3D relationships between the parameters c_1, c_2 and the absorption coefficient μ_a and the scattering coefficient μ_s are presented, respectively.

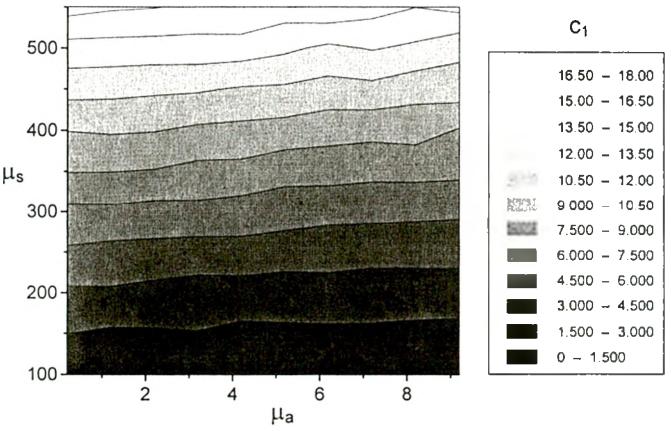

Fig. 6. Correlation between the Groenhuis–Farrell function parameter c_1 and absorption and scattering coefficients for anisotropy factor $g = 0.9$.

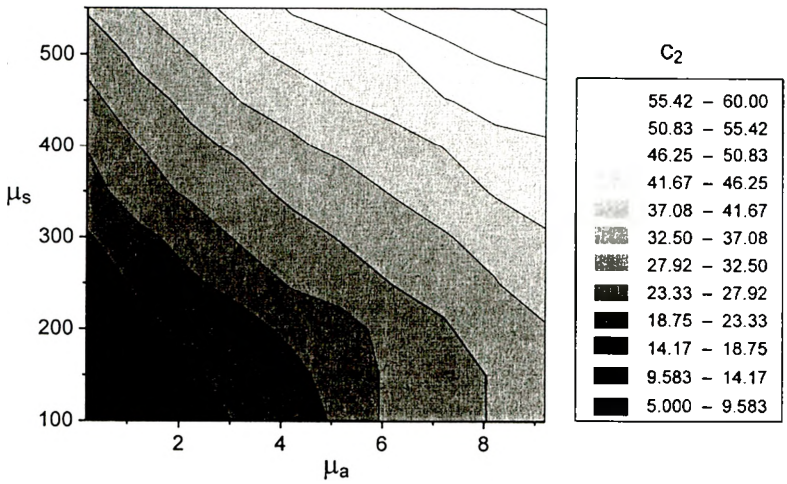

Fig. 7. Correlation between the Groenhuis–Farrell function parameter c_2 and absorption and scattering coefficients for anisotropy factor $g = 0.9$.

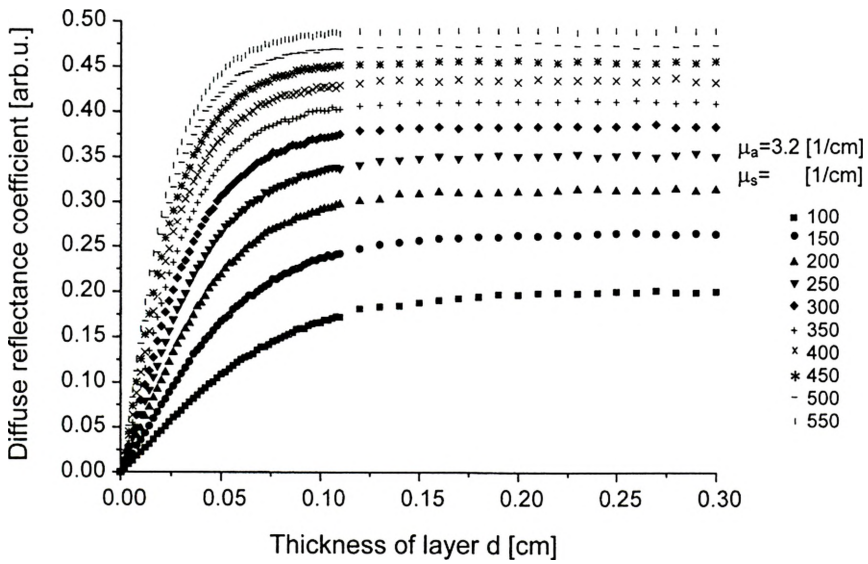

Fig. 8. Diffuse reflectance coefficient *vs* thickness of the first layer for different scattering coefficients ($\mu_s = 100-550$ cm^{-1}) and constant absorption coefficient ($\mu_a = 3.2$ cm^{-1}).

Results obtained in the second series of simulations are presented in Figs. 8 – 11. They include 100 calculations of function $R_d(d)$ obtained for various combinations of coefficients μ_a and μ_s. In Figure 8, the relationships between the diffuse reflectance coefficient and the thickness of the first layer for different scattering coefficients and constant absorption coefficient ($\mu_a = 3.2$ cm^{-1}) are presented. Similar relationships

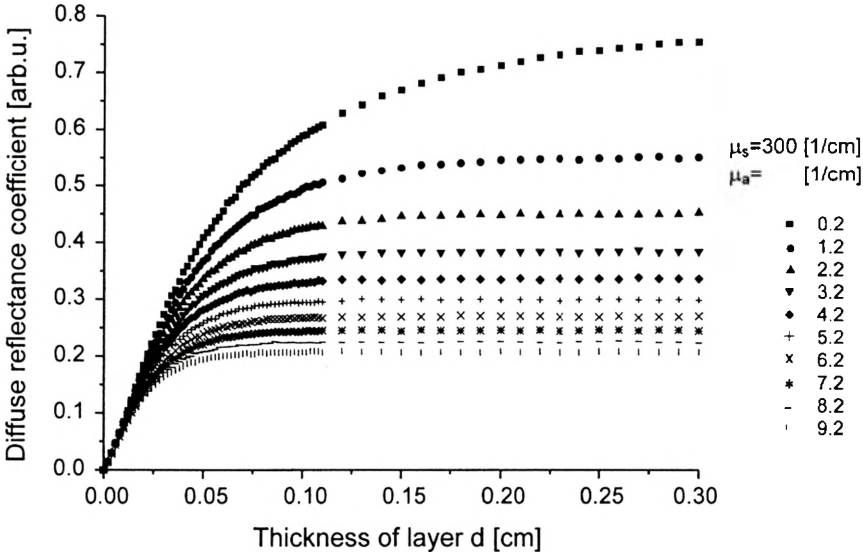

Fig. 9. Diffuse reflectance coefficient *vs.* thickness of the first layer for constant scattering coefficient ($\mu_s = 300$ cm^{-1}) and various absorption coefficients ($\mu_a = 0.2-9.2$ cm^{-1}).

for a constant scattering coefficient ($\mu_s = 300$ cm^{-1}) and various absorption coefficients are presented in Fig. 9. A gradual change of the functions presented in Figs. 8 and 9 is observed. Typical $R_d(d)$ relationships obtained for coefficients $\mu_a = 3.2$ cm^{-1}, $\mu_s = 300$ cm^{-1} and anisotropy factor $g = 0.9$ and the first derivative

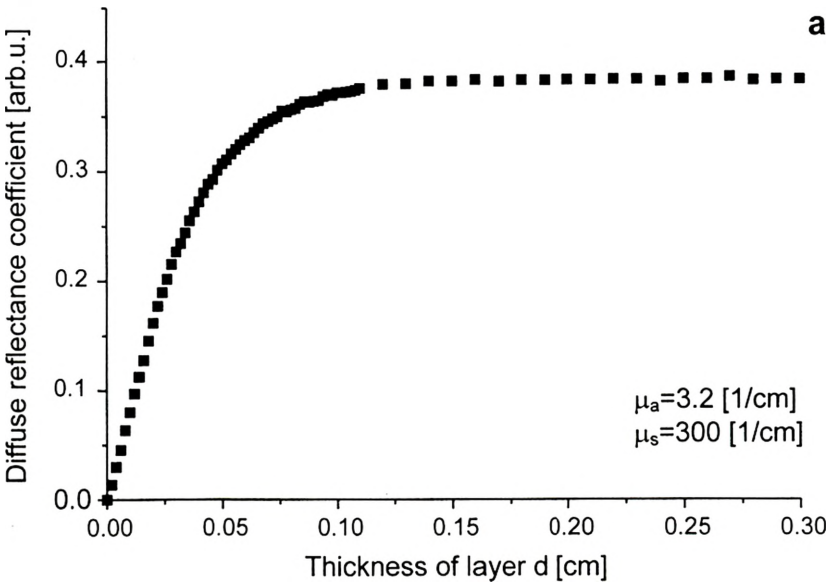

Fig. 10a

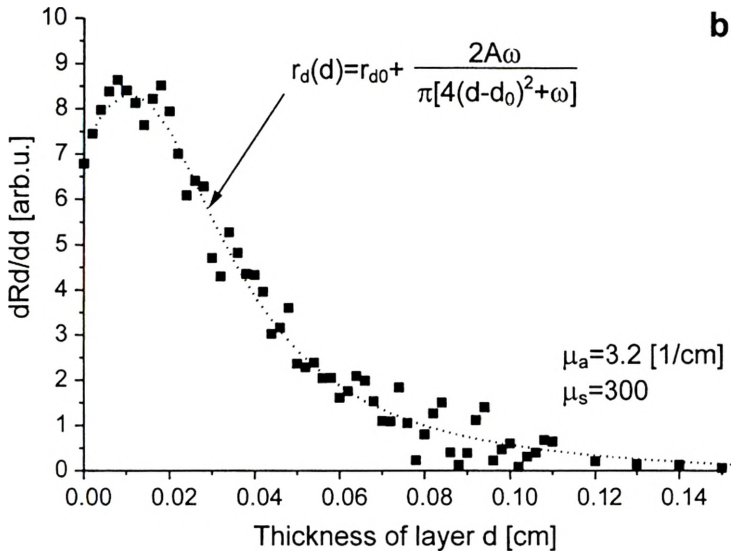

Fig. 10. Diffuse reflectance coefficient *vs.* thickness of the first layer for coefficients $\mu_a = 3.2$ cm^{-1} and $\mu_s = 300$ cm^{-1}, $g = 0.9$ (**a**). First derivative of diffuse reflectance coefficient *vs.* thickness of the first layer for coefficients $\mu_a = 3.2$ cm^{-1} and $\mu_s = 300$ cm^{-1} and anisotropy factor $g = 0.9$ (**b**).

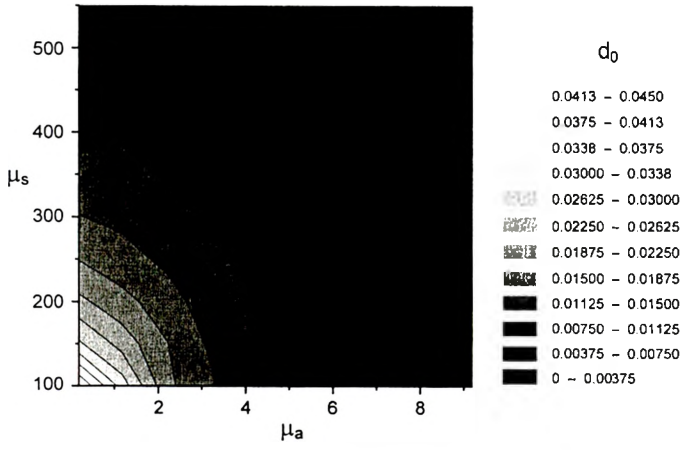

Fig. 11. Correlation between the Lorenz function parameter d_0 and absorption and scattering coefficients for anisotropy factor $g = 0.9$.

$r_d(d)$ of this function are presented in Fig. 10**a**, **b**, respectively. For all derivatives the Lorentz distribution was fitted according to the formula (2) as shown in Fig. 10**b** (examples for selected values of coefficients μ_a and μ_s). Finally, the relationship between coefficients μ_a and μ_s, and the layer thickness d_0 corresponding to maximum of first derivative $r_d(d)$ curve was obtained as presented in Fig. 11.

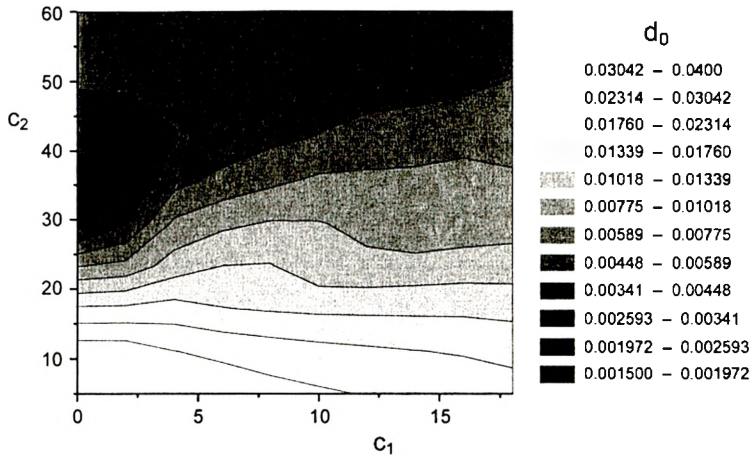

Fig. 12. Relationship between obtained parameters of the diffusely back-scattered light distribution profiles c_1, c_2, and parameter d_0.

The map in Figure 12 represents the overall relationship between the parameters of the diffusely back-scattered light distribution profiles c_1, c_2 and parameter d_0.

Normalized Lorentz functions fitted to derivatives of the simulated diffuse reflectance versus thickness of the first layer as calculated for different distances

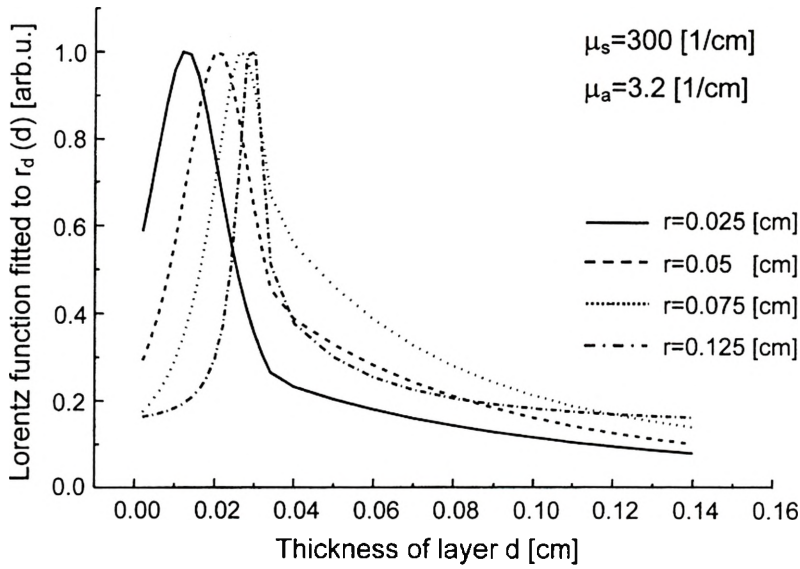

Fig. 13. Normalised derivatives of the diffuse reflectance coefficient *vs.* thickness of the first layer calculated for different distances between the emitter and the detector, and for coefficients $\mu_a = 3.2\ \mathrm{cm}^{-1}$, $\mu_s = 300\ \mathrm{cm}^{-1}$, and anisotropy factor $g = 0.9$.

between the emitter and the detector (for distance r from 0.025 to 0.125 cm), and for coefficients $\mu_a = 3.2\ \mathrm{cm}^{-1}$, $\mu_s = 300\ \mathrm{cm}^{-1}$, and anisotropy factor $g = 0.9$ are shown in Fig. 13. The shift of the maximum position of parameter d_0 as a function of the emitter–detector distance is clearly observed.

4. Discussion and conclusions

The results presented in this study show that the parameters of the diffusely back-scattered light distribution are strongly dependent on the tissue optical properties. This effect was also noticed by other authors [7]–[11].

Many authors have employed the profile of the diffusely back-scattered light distribution for estimation of the light penetration depth [7]–[10], [18]. The formula proposed by Farrell was based on the diffusion equation. However, in case of the low power laser source used it is allowed to detect useful optical signals only at a distance of 0–2 mm from the emitter, but unfortunately, only few studies were performed for short emitter–detector distances ($r < 1.5$ mm) [11], [14], [19], [20].

With the assumption that the tissue within the measured volume is optically homogenous, it is possible to estimate the depth of the scattering volume by the use of the diffusely back-scattered light distribution profile. Recent studies published by NILSSON [21] suggest that the relation between the light intensities detected at two distances from the emitting fibre correlates with the path-length of photons in the tissue.

In our study the simulated relationships show that using the parameters c_1 and c_2 of the diffusely back-scattered light distribution profile, the value of thickness d_0 can be calculated. It is possible to estimate the diffusely back-scattered light distribution profile in practice by the use of multidetector instrumentation [22].

Of further interest is the shift of the maximum position of parameter d_0 with the tissue optical properties presented in Fig. 13. This shift corresponds to different depths of scattering volume for different emitter–detector distances. This observation can be useful in designing the multidistance probes sensitive to scattering volume depths. This phenomenon was previously observed also experimentally in application to the laser-Doppler flowmetry [22]–[25] and investigated theoretically [26], [27].

In summary, the results presented in this paper may be useful for designing probes that allow for quantitative measurement of the depth of light penetration. In future constructions only a few channels for estimation of the diffusely back-scattered light profile will be necessary for coefficients c_1 and c_2 assessment. Signal processing algorithm will allow for parameter d_2 estimation.

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